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APPENDIX D

VERIFICATION AND VALIDATION OF THE EPA'S COMPOSITE MODEL FOR TRANSFORMATION PRODUCTS (EPACMTP), AND ITS DERIVATIVES

D.1 VERIFICATION HISTORY

EPACMTP has been verified extensively by comparing its simulation results against both analytical and numerical solutions. Numerous verification cases were conducted from 1991-2000. A summary of the verification cases is provided in the following subsections. The accompanying Figures for selected test cases are presented in the designated Subappendices.

Subsequent to the verification described below, version 2 of the EPACMTP model (the version of EPACMTP that includes the pseudo-3D aquifer transport option) was tested and verified. The results of this verification are documented in U.S. EPA, 2001.

D.1.1 ORD VERIFICATION (1992-1993)

In 1992, a verification analysis of the newly developed EPACMTP was performed by the Office of Research and Development (ORD) of the US EPA (US EPA, 1992). A list of verification cases in the verification exercise is listed in Table D.1. As shown in the table, two steps of code verification were conducted: a re-verification of the original test problems and data files provided by HydroGeoLogic, Inc. and independent verification using alternative test criteria. Based on the analysis of Tetra Tech, some technical limitations in the EPACMTP code were identified. One of the weaknesses, which occurred in the aquifer module, pertained to potential mass loss of contaminants from the system due to the upstream boundary proximity and conditions in EPACMTP. The code was modified in response to the comments (HydroGeoLogic, Inc., 1993).

D.1.2 MODULE-LEVEL VERIFICATION (1993-1994)

A module-level verification task was performed between 1993-1994 and reported in EPACMTP Background Documents (US EPA, 1996 b, d). Numerous components of EPACMTP's flow and transport sub-modules, in both the vadose and aquifer modules, were verified between 1993-1994 against analytical solutions, and numerical solutions from a number of simulators with similar mathematical frameworks. Details of the verification are presented below.

D.1.2.1 Vadose-Zone Module Verification

The vadose-zone and the aquifer modules were subdivided into the flow and transport sub-modules. The ten verification cases for the vadose-zone module are summarized in Table D.2 and are briefly described below. Excerpts of verification results for the vadose-zone test cases are presented in figures in Subappendix D.A. Reference to the figures in Subappendix D.A is provided in Table D.2. Additional information regarding the test cases and respective verification results may be found in US EPA (1996b). The

Table D.1 Summary of EPACMTP Verification by the Office of Research and Development, U.S. EPA, and Tetra Tech, Inc. in 1992-1993 (from US EPA, 1992)

Case	Description	Reverification of HGL Tests	Independent Verification
1	Steady-state, aquifer flow, single layer	Yes	Yes
2	Steady-state, vadose-zone transport, two layers		Yes
3	Transient vadose-zone transport, single layer - analytical solution	Yes	Yes
4	Transient vadose-zone transport, single layer - numerical solution		Yes
5	Transient vadose-zone transport, single layer, non-conservative solute - numerical solution		Yes
6	Transient vadose-zone transport, three layers, non-conservative solute - numerical solution		Yes
7	Transient vadose-zone transport, single layer, nonlinear adsorption - numerical solution	Yes	
8	Multiple species transport; 3-member chain decay; source decay	Yes	
9	Steady-state, aquifer flow	Yes	Yes
10	Quasi-3D aquifer transport - numerical solution	Yes	Yes
11	Non-linear aquifer transport	Yes	Yes
12	3-species transport, 2-D (x,y)	Yes	Yes
13	7-species transport, 2-D (x,y)	Yes	Yes
14	Full-3D aquifer flow and transport	Yes	

vadose-zone module of EPACMTP was originally called FECTUZ. The numerical transport simulation in FECTUZ is no longer part of EPACMTP.

The first three test cases of the vadose-zone module are for the flow sub-module and focus on steady-state flow within layered and non-layered soils. They were verified by comparing the results of the semi-analytical FECTUZ (US EPA, 1989) module against the numerical finite element VADOFT model (Huyakorn, et al., 1987). Test Case 1 evaluated steady-state infiltration in a soil. Test Cases 2 and 3 are similar, both involving steady-state infiltration in a layered soil, whereas Test Case 3 introduced the surface impoundment boundary condition (ponding depth) to the system.

The last seven test cases, summarized in Table D.2, pertain to transport sub-module verification. Test Cases 4 and 5 tested the analytical steady-state transport module and the semi-analytical transport solution, respectively. Test Case 4 involved steady-state transport in a layered soil and verification against the FECTUZ numerical solution, while Test Case 5 evaluated transient transport with verification against both the FECTUZ numerical solution and the HYDRUS code (Kool and van Genuchten, 1991).

Test Cases 6 through 10 utilize the FECTUZ numerical solution to examine transport of a contaminant in a soil column. Case 6 concerns 1-D transport of a conservative solute species and is verified against the analytical solution of Ogata and Banks (1961). Test case 7 considers downward vertical transport of both conservative and non-conservative constituents. The results are compared against the analytical solution given by van Genuchten and Alves (1982). Test Case 8 concerns 1-D transport of a conservative solute species in a layered soil column. Two sub-cases with different dispersivity values were compared with the analytical solutions presented by Shamir and Harlemann (1967) and Hadermann (1980). Test Case 9 considers solute transport with both linear and nonlinear adsorption. This is verified against the MOB1 finite element solution (van Genuchten and Alves, 1982). Test Case 10 examines transport of a 3-member, straight decay chain and is verified against the analytical solution, modified from Hodgkinson and Maul (1985).

D.1.2.2 Aquifer Module Verification

The saturated zone module of EPACMTP was originally developed on a stand alone basis and called CANSAZ-3D. Seven benchmark problems were analyzed to verify the flow and transport solutions in the CANSAZ-3D modules; (Sudicky et al, 1990) and are summarized in Table D.3. Excerpts of verification results for the test cases are presented in Subappendix D.B. Reference to the figures in Subappendix D.B is provided in Table D.3. Additional information regarding the test cases and respective verification results may be found in U.S. EPA (1996b). Test Case 1 was designed to verify the 3-D steady-state groundwater flow solution. For this purpose, the hydraulic head and groundwater flow velocities obtained from CANSAZ-3D were compared against the MNDXYZ analytical solution (Ungs, 1986; Appendix B of U.S. EPA, 1996b). Test Case 2 was designed to compare the analytical and numerical transport solutions for the case of single species transport in a uni-directional steady-state groundwater flow field. Test Case 3 involved two-dimensional transport of a 3-member decay chain. The CANSAZ-3D results for this test problem were verified against the numerical VAM2D code (Huyakorn et al., 1992). Test Case 4 involved verification of CANSAZ-3D against an analytical solution (Sudicky et al., 1991) for a case involving a complex, seven-member branched decay chain. Test Case 5 was designed to verify the nonlinear sorption option. This problem involves 1-D flow and transport with a nonlinear Freundlich isotherm. CANSAZ-3D was verified against the numerical MOB1 (van Genuchten, 1981) and FECTUZ. Test Case 6 involves fully 3-D flow and transport. The CANSAZ-3D solution was compared against results obtained with the 3-D DSTRAM flow and transport code (Huyakorn, et al., 1994). Test Case 7 was designed to evaluate

Table D.2 Verification Cases for the Vadose-Zone Module (1993-1994)

Case	Description	Verification Method	Excerpts of Verification Results Presented in
1	Steady-state infiltration	Semi-analytical FECTUZ module vs. fully numerical finite element VADOFT	Figure D.A.1, Subappendix D.A
2	Steady-state infiltration in a layered soil	Semi-analytical FECTUZ module vs. fully numerical finite element VADOFT	Figure D.A.2, Subappendix D.A
3	Steady-state infiltration in a layered soil with a ponding depth	Semi-analytical FECTUZ module vs. fully numerical finite element VADOFT	Figure D.A.3, Subappendix D.A
4	Steady-state transport in a layered soil	Steady-state analytical solution vs. finite element numerical solution of FECTUZ	Figure D.A.4, Subappendix D.A
5	1-D transient transport under pulse input conditions	Semi-analytical solution vs. numerical finite element module of FECTUZ and the HYDRUS code	Figure D.A.5, Subappendix D.A
6	1-D transport of a conservative solute species in a saturated soil column of semi-infinite length	Numerical solution of FECTUZ vs. analytical solution of Ogata and Banks (1961)	Figure D.A.6, Subappendix D.A
7	1-D transport of a conservative and non-conservative solute species in a saturated soil column of finite length	FECTUZ vs. analytical solution of van Genuchten and Alves (1982)	Figure D.A.7, Subappendix D.A
8	Transport of a conservative species in a layered soil column	FECTUZ vs. Shamir and Harleman (1967) and Hadermann (1980)	Figures D.A.8 and D.A.9, Subappendix D.A
9	Transient transport under conditions of nonlinear adsorption with a pulse source	FECTUZ vs. finite difference code MOB1	Figure D.A.10, Subappendix D.A
10	Multispecies transport with three member, straight decay chain with a decaying source boundary condition	FECTUZ vs. analytical solution modified from Hodgkinson and Maul (1985)	Figure D.A.11, Subappendix D.A

Table D.3 Verification Cases for the Saturated Zone Module (1993-1994)

Case	Description	Verification Method	Excerpts of Verification Results Presented in
1	Steady-state groundwater flow in a 3-D domain	CANSAZ-3D vs. analytical solution of MNDXYZ	Figure D.B.1, Subappendix D.B
2	Single species transport in a uni-directional flow field - analytical and numerical transport modules	CANSAZ-3D vs. 3-D analytical solution	Figure D.B.2, Subappendix D.B
3	2-D transport of a 3-member decay chain. Steady-state flow and transient solute transport in an unconfined aquifer	CANSAZ-3D vs. VAM2D	Figure D.B.3, Subappendix D.B
4	2-D transport of a complex, seven-member branched decay chain with 1-D groundwater flow	CANSAZ-3D vs. Gaussian source analytical solution of Sudicky et al. (1991)	Figure D.B.4, Subappendix D.B
5	Nonlinear sorption reactions in a 1-D, steady-state flow and transient transport. Pulse source using a Freundlich isotherm	CANSAZ-3D vs. MOB1 and FECTUZ	Figure D.B.5, Subappendix D.B
6	Steady-state flow and transport modeling of a single conservative species in 3-D aquifer domain	CANSAZ-3D vs. DSTRAM	Figure D.B.6, Subappendix D.B
7	Steady-state groundwater flow and transient solute transport in 3-D aquifer domain with a horizontal patch source	CANSAZ-3D vs. VAM3D	Figure D.B.7, Subappendix D.B

the automatic model domain discretization option for a 3-D flow and transport problem and was verified against the numerical VAM3D code (Panday et al., 1993).

D.1.2.3 Metals Transport Module

The major modifications to accommodate metals transport with nonlinear sorption were made to the vadose-zone module, therefore the verification cases are applicable to this module. Five verification test cases are summarized in Table D.4 and excerpts of verification results are presented in Subappendix D.C. Reference to the figures in Subappendix D.C is provided in Table D.4. Additional information regarding the test cases and respective verification results may be found in U.S. EPA (1996d). Test Case 1 involved continuous release of a non-sorbing solute to test the linear adsorption partitioning capabilities. An analytical solution from Ogata (1970) was compared against the EPACMTP results. Test Case 2 involved nonlinear Freundlich adsorption isotherms. The Freundlich isotherm was represented by its closed form. Two different source conditions were utilized: continuous and finite sources. Freundlich exponents greater than and less than one were examined. The results from EPACMTP were compared with those from HYDRUS. Test Case 3 involves transport of lead in a fully saturated soil column. The verification of this case was performed by comparing the computed cumulative mass against the total input mass. Test Case 4 involves 1-D transport of a solute, with Freundlich exponents of less than and greater than one and was verified against HYDRUS.

D.1.3 VERIFICATION OF INDIVIDUAL MODULES AND A COMPOSITE MODEL IN EPACMTP (1997)

In 1997, a testing plan was developed for EPACMTP code verification (US EPA, 1997), in accordance with the ASTM, “Standard Guide for Developing and Evaluating Ground-Water Modeling Codes” (ASTM, 1996). The verification process focused on a single problem geometry, representative of waste disposal scenarios in terms of spatial dimensionality and climatic/hydrogeological conditions. The verification process first subdivided the problem setting into individual hydrogeologic components, assessed their functionality relative to an overall fate and transport problem, and then compared each component to analytical solutions or other codes.

The vadose-zone module, the aquifer module, and the composite model were verified following the ASTM standards. The vadose-zone problem geometry was a 1-D column extending from the land surface to the water table. Boundary conditions for numerical contaminant transport involved a continuous source on the water table beneath the waste management unit. The region of the water table outside the source area received constant recharge from the ground surface. Ten test cases were conducted. These test cases may be subdivided into those for the vadose-zone module, the aquifer module, and the composite model, and are summarized in Tables D.5a, D.5b, and D.5c, respectively.

Table D.4 Verification Cases for Metals Transport in the Vadose-Zone (1993-1994)

Case	Description	Verification Method	Excerpts of Verification Results Presented in
1	Linear adsorption partitioning with continuous release of a non-sorbing solute	Analytical solution (Ogata, 1970) vs. EPACMTP result	Figure D.C.1, Subappendix D.C
2	Nonlinear adsorption isotherm. The Freundlich isotherm was represented by its closed function form. Freundlich isotherms greater than and less than one were considered for continuous and finite source conditions	EPACMTP vs. HYDRUS	Figures D.C.2 and D.C.3, Subappendix D.C
3	Transport of lead using MINTEQA2-generated isotherms	Cumulative vs. total input mass	Figure D.C.4, Subappendix D.C
4	Pulse source and Freundlich exponents of 0.5, 0.8, and 1.5	Analytic solution vs. HYDRUS	Figure D.C.5, Subappendix D.C

Table D.5a Verification Cases for the Vadose-Zone Module (1997)

Case	Description	Verification Method	Excerpts of Verification Results Presented in
1	Steady-state variably saturated flow	EPACMTP vs. STAFF3D	Figure D.D.1, Subappendix D.D
2	Infiltration through a clay liner from a surface impoundment	EPACMTP vs. STAFF3D	Figure D.D.2, Subappendix D.D
3	Contaminant transport with linear sorption and decay	Numerical EPACMTP vs. analytical EPACMTP	Figure D.D.3, Subappendix D.D
4	Contaminant transport with branched chain decay and linear sorption	EPACMTP vs. VAM2D	Figure D.D.4, Subappendix D.D

Table D.5b Verification Cases for the Aquifer Module (1997)

Case	Description	Verification Method	Excerpts of Verification Results Presented in
5	3-D steady-state groundwater flow	EPACMTP vs. MNDXYZ analytical solution	Figure D.E.1 and D.E.2, Subappendix D.E
6	3-D contaminant transport with linear sorption and decay	EPACMTP numerical module vs. EPACMTP analytical module; EPACMTP vs. VAM3DF	Figure D.E.3, Subappendix D.E
7	3-D contaminant transport with four species, branched chain decay and linear sorption	EPACMTP vs. STAFF3D	Figure D.E.4, Subappendix D.E

Table D.5c Verification Cases for Composite Module (1997)

Case	Description	Verification Method	Excerpts of Verification Results Presented in
8	Composite flow and contaminant transport	EPACMTP vs. VAM3DF	Figure D.F.1, Subappendix D.F
9	Monte Carlo analysis based on composite flow and contaminant transport	EPACMTP vs. VAM3DF	Figure D.F.2, Subappendix D.F

D.1.3.1 Vadose-Zone Module Verification

The vadose-zone module verification is summarized with four cases in Table D.5a and excerpts of verification results are presented in Subappendix D.D. Reference to the figures in Subappendix D.D is provided in Table D.5a. Additional information regarding the test cases and respective verification results may be found in U.S. EPA (1997). Test Case 1 evaluated steady-state variably saturated flow and Test Case 2 considers infiltration through a clay liner and ponding depth. Test Cases 3 and 4 both considered contaminant transport with linear sorption, but Test Case 3 examined linear decay while Test Case 4 evaluated four species with branched chain decay. Test Cases 1 and 2 were verified against STAFF3D (HydroGeoLogic, Inc., 1995a), Test Case 4 was verified against VAM2D while Test Case 3 compared the steady-state results from numerical and analytical transport modules of EPACMTP.

D.1.3.2 Aquifer Module Verification

The aquifer module verification is summarized with three cases in Table D.5b and excerpts of verification results are shown in Subappendix D.E. Reference to the figures in Subappendix D.E is provided in Table D.5b. Additional information regarding the test cases and respective verification results may be found in U.S. EPA (1997). The 3-D steady-state fully saturated flow module in EPACMTP was verified against the analytical solution MNDXYZ in Test Case 5. Test Cases 6 and 7 examined contaminant transport and were verified against VAM3DF (HydroGeoLogic, Inc., 1995b) and STAFF3D, respectively. Test Case 6 involved transport of a contaminant with linear sorption and decay, while Test Case 7 involved linear sorption and a four species, branched chain decay.

D.1.3.3 Composite Model Verification

The EPACMTP composite model comprises the following fate and transport modules: a vadose-zone module, and a aquifer (saturated zone) module. These modules are connected according to the detailed description in US EPA (1996). The composite model verification is summarized with two test cases in Table D.5c and excerpts of verification results are shown in Subappendix D.F. Reference to the figures in Subappendix D.F is provided in Table D.5c. Additional information regarding the test cases and respective verification results may be found in U.S. EPA (1997). Test Case 8 considered the composite flow and contaminant transport structure. Test Case 9 assessed the sensitivity of the geometric assumptions used to develop EPACMTP. A limited Monte-Carlo analysis was performed to assess the sensitivity of the confined water table assumption to predicting the probability of exceedance at a monitoring well. Both Test Cases 8 and 9 were verified against VAM3DF which is a 3D, variably saturated numerical flow and transport code.

Table D.6a Verification Cases for the 3MRA Vadose-Zone Module (1999)

Case	Description	Verification Method	Excerpts of Verification Results Presented in
1	Exponentially depleting conservative source with no sorption or hydrolysis	Vadose-Zone Module vs. EPACMTP	Figure D.G.1, Subappendix D.G
2	Constant-concentration source pulse with no sorption or hydrolysis	Vadose-Zone Module vs. EPACMTP	Figure D.G.2, Subappendix D.G
3	Constant-concentration source pulse with sorption and hydrolysis, one species	Vadose-Zone Module vs. EPACMTP	Figure D.G.3, Subappendix D.G
4	Constant-concentration source pulse with sorption and hydrolysis, and chain decay	Vadose-Zone Module vs. EPACMTP	Figure D.G.4, Subappendix D.G
5	Metals: (Mercury, and Lead), with constant-concentration source pulse with MINTEQ-based sorption and no hydrolysis	Vadose-Zone Module vs. EPACMTP	Figures D.G.5 and D.G.6, Subappendix D.G
6	Constant-concentration source pulse with biodegradation, sorption and chain decay	Vadose-Zone Module vs. EPACMTP	Figure D.G.7, Subappendix D.G
7	1-D contaminant transport between a top boundary at the bottom of the source zone and the water table with mass loading to the top boundary from the leachate flux from the source module	Vadose-Zone Module vs. MODFLOW-SURFACT	Figure D.G.8, Subappendix D.G
8	1-D variable saturated flow between a top boundary at the bottom of the source zone and the water table with mass loading to the top boundary from the leachate flux from the source module	Vadose-Zone Module vs. MODFLOW-SURFACT	Figure D.G.9, Subappendix D.G

Table D.6b Verification Cases for the 3MRA Aquifer Module (1999)

Case	Description	Verification Method	Excerpts of Verification Results Presented in
1	Exponentially depleting source with no sorption or hydrolysis	Aquifer Module vs. EPACMTP	Figure D.H.1, Subappendix D.H
2	Constant-concentration source pulse with no sorption or hydrolysis	Aquifer Module vs. EPACMTP	Figure D.H.2, Subappendix D.H
3	Constant-concentration source pulse with sorption and hydrolysis, one species	Aquifer Module vs. EPACMTP	Figure D.H.3, Subappendix D.H
4	Constant-concentration source pulse with sorption and hydrolysis, and two species with chain decay	Aquifer Module vs. EPACMTP	Figures D.H.4 and D.H.5, Subappendix D.H
5	Metals: (Mercury, and Lead), with constant-concentration source pulse with sorption and no hydrolysis	Aquifer Module vs. EPACMTP	Figure D.H.6, Subappendix D.H
6	Constant-concentration source pulse with biodegradation, sorption and four species chain decay	Aquifer Module vs. EPACMTP	Figures D.H.7, D.H.8, D.H.9, and H.10, Subappendix D.H
7	Comparison of Monte Carlo saturated zone simulations	Aquifer Module vs. EPACMTP	Figure D.H.11, Subappendix D.H

Table D.6c Verification Cases for the 3MRA Pseudo-Three Dimensional Aquifer Module (1999)

Case	Description	Verification Method	Excerpts of Verification Results Presented in
1	Average Groundwater Specific Flow Rate	Aquifer Module vs. Darcy's Law analytical solution	Figure D.I.1, Subappendix D.I
2	Numerical Component of the Contaminant Transport Sub-module	Aquifer Module vs. analytical solution by Ogata	Figure D.I.2, Subappendix D.I
3	Analytical-Numerical Component of the Contaminant Transport Sub-module	Aquifer Module vs. analytical solution	Figure D.I.3, Subappendix D.I

D.1.4 VERIFICATION OF 3MRA SUBSURFACE FLOW AND TRANSPORT MODULES (1999)

In 1999, the flow and transport components for the vadose-zone module and aquifer module were extracted from EPACMTP to provide the groundwater pathway module for the multi-media, multi-pathway, and multiple receptor risk assessment modeling system (3MRA). The basic premise for verification of the vadose-zone and aquifer modules was that EPACMTP had been rigorously verified, so it was sufficient to show that the modules reproduced EPACMTP results. Therefore, both the steady-state flow and transport sub-modules of the aquifer module (US EPA, 1999c) and the flow and transport sub-modules of the vadose-zone module (US EPA, 1999b,c) were compared against the numerical results from EPACMTP to ensure that the extracted modules remained intact. There are two exceptions that will be discussed below. The new saturated zone pseudo-3D module was also developed during this period (US EPA, 1999a).

The eighteen test cases for the vadose-zone, aquifer, and pseudo 3-D modules are summarized in Tables D.6a, D.6b, and D.6c, respectively. The figures are presented in Subappendix D.G through D.I. The vadose-zone problem geometry was a 1-D column extending from the land surface to the water table. Boundary conditions for numerical contaminant transport involved a continuous source on the water table beneath the waste management unit. The region of the water table outside the source area was also considered to be a recharge boundary.

D.1.4.1 Vadose-Zone Module Verification

There are eight vadose-zone module verification cases (Table D.6a). Excerpts of results for the verification cases are presented in Subappendix D.G. Reference to the figures in Subappendix D.G is provided in Table D.6a. Additional information regarding the test cases and respective verification results may be found in U.S. EPA (1999b,c). All of the cases concern contaminant transport. Test Case 1 evaluated an exponentially depleting source. Test Case 2 involved transport of a contaminant with no sorption and no hydrolysis. Test Case 3 examined sorption and hydrolysis with one species, while Test Case 4 involved two species with chain decay. Test Case 5 examined linear and nonlinear metal transport using the MINTEQA2 isotherms. Test Case 6 evaluated biodegradation resulting in chain decay reactions with four species. Test Cases 7 and 8 examined contaminant concentration at a receptor well and pressure heads at each grid node, respectively. In this instance, both Test Case 7 and 8 were verified against MODFLOW-SURFACT (HydroGeoLogic, Inc., 1996), a three-dimensional numerical groundwater flow and transport code.

D.1.4.2 Aquifer Module Verification

There are seven aquifer module verification cases (Table D.6b) with excerpts of verification results presented in Subappendix D.H. Reference to the figures in Subappendix D.H is provided in Table D.6b. Additional information regarding the test cases and respective verification results may be found in U.S. EPA (1999c).

Table D.7a Verification Cases for the 3MRA Vadose-Zone Module (2000)

Test Area	General Requirements	Number of Verification Cases	Excerpts of Verification Results Presented in
1	Verification of reading and screening of source and site- specific input data	3	N/A
2	Verification of pre-simulation processing of input data	2	N/A
3	Verification of the flow component	1	N/A
4	Verification of the non-metals transport component	5	Figure D.J.1, Subappendix D.J
5	Verification of the metals transport component	4	Figure D.J.2, Subappendix D.J
6	Verification of post simulation output	2	N/A
7	Verification of the vadose-zone module’s robustness	13	N/A

Table D.7b Verification Cases for the 3MRA Aquifer Module (2000)

Test Area	General Requirements	Number of Verification Cases	Excerpts of Verification Results Presented in
1	Verification of reading and screening of source and site-specific input data	4	N/A
2	Verification of pre-simulation processing of input data	17	N/A
3	Verification of the fractured media component	3	N/A
4	Verification of the heterogeneous saturated media component	1	N/A
5	Verification of reading and screening of chemical-specific, biodegradation, and metal-specific data	6	N/A
6	Verification of numerical grid generation	4	N/A
7	Verification of the flow component	4	N/A
8	Verification of the contaminant fate and transport component	19	Figures D.K.1 and D.K.2, Subappendix D.K
9	Verification of the aquifer module's robustness	11	N/A

Test Case 1 evaluated an exponentially depleting source. Test Case 2 involved transport of a conservative contaminant with no sorption and no hydrolysis. Test Case 3 examined sorption and hydrolysis with one species, while Test Case 4 involved two species with chain decay. Test Case 5 examined linear and nonlinear metal transport using the MINTEQA2 isotherms. Test Case 6 evaluated biodegradation resulting in chain decay reactions with four species. Test Case 7 evaluated the generated Monte Carlo distributions.

D.1.4.3 Pseudo-3D Module Verification

There are three verification cases for the pseudo-3D aquifer module (Table D.6c). Excerpts of verification results are shown in Subappendix D.I. Reference to the figures in Subappendix D.I is provided in Table D.6c. Additional information regarding the test cases and respective verification results may be found in U.S. EPA (1999a,c). Test Case 1 examined the average groundwater specific flow rate determined by the saturated flow sub-module and was verified using Darcy's Law. Test Case 2 examined the numerical component of the contaminant transport sub-module and is verified using the analytical solution by Ogata (1970). Test Case 3 verified the combined analytical-numerical contaminant transport sub-module using verification results of Test Case 2 subject to the analytical portion of the aquifer transport sub-module.

D.1.5 COMPREHENSIVE VERIFICATION OF THE 3MRA VADOSE-ZONE AND PSEUDO-3D AQUIFER MODULES (2000)

In 2000, a comprehensive verification was conducted of all of the components in the extracted aquifer and the vadose-zone modules (US EPA, 2000 a,b). For testing purposes, each component was executed as a stand-alone program outside of the 3MRA Software System environment.

D.1.5.1 Vadose-Zone Module Verification

There are 40 vadose-zone module verification test cases summarized in Table D.7a. Selected figures for Test Areas 4 and 5, the non-metals and metals transport components, are presented in Subappendix D.J. Reference to the figures in Subappendix D.J is provided in Table D.7a. Additional information regarding the test cases and respective verification results may be found in U.S. EPA (2000a). The reading and screening of source and site-specific input data was verified in 3 cases. Verification of the pre-simulation processing of input data was performed with 2 cases. The flow, non-metal transport, and metals transport components were verified with 1, 5 and 4 cases, respectively. The post simulation processing of output data was verified with 2 cases. The robustness testing verified the stability of the simulation when executed with extreme values for selected parameters. The parameters were selected based on the results of a parameter sensitivity analysis (U.S. EPA, 1996e). The vadose-zone module's robustness was verified with 13 cases.

D.1.5.2 Aquifer Module Verification

There are 69 aquifer module verification cases summarized in Table D.7b. Selected figures for Test Area 8, the fate and transport component, are present in Subappendix D.K. Reference to the figures in Subappendix D.K is provided in Table D.7b. Additional information regarding the test cases and respective verification results may be found in U.S. EPA (2000b). The reading and screening of source and site-specific input data was verified in 4 cases. Verification of the pre-simulation processing of input data was performed with 17 cases. The fractured media, and heterogeneous saturated media components were verified with 3, and 1 cases, respectively. The reading and screening of chemical-specific, biodegradation and metal-specific data was verified in 6 tests. The numerical grid generation was verified in 4 cases. The flow component was verified with 4 cases, while the contaminant fate and transport component was verified in 19 cases. The robustness testing verified the stability of the simulation when executed with extreme values for selected parameters. The parameters were selected based on the results of a parameter sensitivity analysis (U.S. EPA, 1996e). The aquifer module's robustness was verified with 11 cases.

D.2 VALIDATION HISTORY

Validation, as defined previously, may be conducted using actual measured field data. It is helpful to assess the validity of simplifying assumptions and the predictive capabilities of EPACMTP against well documented realistic site data. EPACMTP and its predecessors (from which flow and transport components in EPACMTP were derived) have been validated based on actual observations at four sites, although no validation has been performed using the 3MRA vadose-zone and aquifer zone modules. In 1990, EPACMS (CANSAZ) was validated against the data from the Borden Landfill site, along with the data from a second agricultural field site on Long Island, New York (US EPA, 1990). This validation included the combination of the saturated and the vadose-zone modules in EPACMS. In 1993, the composite model was validated against data from a Dodge City, Kansas site (Kool et al., 1994). Then, in 1995 EPACMTP was validated against the data from the EBOS Site 24 in New York (US EPA, 1995). The four validation cases are presented in the following subsections. Note that all the figures that are referenced to in the following subsections are presented in Subappendix D.L.

D.2.1 BORDEN SITE

The Borden landfill is located in Borden, southern Ontario, Canada, and occupies an area of approximately 4 ha (Figure D.L.1). The landfill was operational for 36 years and at its closure was capped with a thin layer of sand. The site overlies 8 to 20 meters of a glaciofluvial sand aquifer, which overlies a confining silty clay deposit. The chloride plume extends about 700 m northward of the landfill and occupies nearly the entire vertical thickness of the aquifer. The waste material was deposited just above the water table, therefore transport did not occur in the vadose-zone.

Generally, the flow and transport parameters and the procedure described by Frind and Hokkanen (1987) were used for the EPACMS simulation. The exception is that Frind and Hokkanen assigned a higher recharge rate to some areas outside of the source area, but this refinement was not utilized for the EPACMS simulation. A curvilinear grid was utilized to describe the aquifer geometry and because EPACMS assumes a constant saturated thickness, the VAM3D-CG code (Huyakorn and Panday, 1989) was used to perform the groundwater flow simulation. Next, the CANSAZ (EPACMTP module) module was used to simulate transient transport. CANSAZ utilized the same finite grid as the groundwater flow simulation, as well as the groundwater velocity distribution from the VAM3D simulation.

The chloride concentrations were compared for the observed values (Figure D.L.2), the CANSAZ simulation values (Figure D.L.3) and the Frind and Hokkanen simulation values (Figure D.L.4). The CANSAZ model accurately predicted the extent of the plume and the overall plume shape compared to both the Frind and Hokkanen model and the field values.

D.2.2 LONG ISLAND SITE

The site is located on the south shore of the North Fork of Long Island, New York (Figure D.L.5). The agricultural site was contaminated with the pesticide aldicarb in the 1970’s. The source was a 2.5 ha potato field overlying sandy loam soils with a high infiltration rate. An unconfined aquifer is located approximately 2 meters below the surface.

Both site specific data and monitoring data are limited at this site. The site characterization was obtained from previous studies by INTERA (1980) and Carsel et al. (1985). The EPA Pesticide Root Zone Model (PRZM) (Carsel et al, 1984) was used to predict the 3-year average recharge rate and average aldicarb concentration at the base of the root zone as input for the EPACMS vadose-zone module. The steady-state groundwater flow field was generated using the analytical 2-D solution on EPACMS, followed by a three-year transient aldicarb transport simulation.

The simulated concentrations of aldicarb in groundwater with distance from the source were compared with the observed values (Figure D.L.6). The agreement between the simulated and observed concentrations was quite reasonable, with the relative error decreasing with increasing distance from the source.

D.2.3 DODGE CITY SITE

The Dodge City, Kansas site (Figure D.L.7), located in the Arkansas River valley, is documented by Ourisson et al. (1992). The source is a controlled release of Triasulfuron pesticide (non-conservative) and bromide (conservative) which, over a 2 year period, is transported through the vadose-zone and the aquifer. The site covers an area of approximately 2.3 acres (approximately 1 ha) overlying one meter of sandy loam soil which overlies a sand and gravel unit. The water table is located at a depth of three meters.

The Dodge City site was well characterized, the source was well defined and the monitoring data were available for both soil and groundwater. Site specific values were obtained from Ourisson et al., (1992), Carsel and Parrish (1988), Gelhar et al. (1985), Carsel et al. (1984), and derived values. EPACMTP was used to simulate the flow and transport of both conservative and non-conservative constituents.

The groundwater concentration model predictions were compared against the observed values. The model tended to underestimate bromide concentrations (Figure D.L.8) slightly and overestimate Triasulfuron concentrations (Figure D.L.9). The application of the model to the Kansas field site showed reasonably good agreement between model predictions and groundwater monitoring results.

D.2.4 EBOS SITE

The EPRI research site referred to as EBOS site 24 is a disposal site for a coal tar Manufacturing Gas Plant located in New York state (Figure D.10.). Initially, the coal tar was disposed of in a trench on the site, then over time migrated downward into the aquifer (Figure D.L.11 and D.L.12). The site is characterized by 15 to 30 feet of typical glacial outwash sand deposits overlying a clay confining layer. Napthalene was labeled the constituent of concern, since it was the polyaromatic hydrocarbon (PAH) with the highest concentrations in the coal tar.

The site specific parameters were provided by the Electric Power Research Institute in 1993 and consisted of both known and estimated values. EPACMTP was used to simulate the flow and transport of constituents through the vadose-zone and the aquifer. One point to note was that since the coal tar had moved down into the aquifer, the constituents could be leached out through direct contact with ambient groundwater. In the EPACMTP simulation, it was necessary to leach the constituents out of the waste by infiltration from the vadose-zone.

Napthalene concentrations near the source before (Figure D.L.13) and after (Figure D.L.14) source removal were predicted by EPACMTP. The results from EPACMTP were qualitatively similar to the observed concentration in terms of groundwater concentrations near the source.

D.3 SUMMARY

EPACMTP, its predecessors (EPACMS, CANSAZ, and FECTUZ), and its derivatives (3MRA vadose-zone and aquifer modules) have been verified extensively during the past decade at each of the developmental stages. The model has been verified, in numerous cases, by comparing the simulation results against both analytical and numerical solutions. Additionally, EPACMTP and its predecessors have been validated using actual site data from four different sites. The relevant verification and validation history, discussed in the previous sections of this document, is summarized below.

The preliminary verification of EPACMTP was performed by ORD in 1992. Following the preliminary verification, detailed module-level verification was conducted on the flow and transport sub-modules of the vadose-zone and the aquifer modules between 1993-1994. The modules were verified against analytical solutions, and numerical solutions from a number of well-documented simulators. In 1997, the EPACMTP code was verified utilizing a testing plan developed according to ASTM standards. The vadose-zone and the aquifer modules, as well as the composite model (based on the sequentially linked vadose-zone and aquifer modules), were verified against analytical and numerical solutions. In 1999, the vadose-zone and aquifer modules were extracted from EPACMTP to be included as part of the multi-media, multi-receptor, and multi-pathway risk assessment (3MRA) software system. The flow and transport sub-modules of both modules were verified against the results from EPACMTP. Additionally, for the 3MRA software system a pseudo-3D aquifer module was developed. An exhaustive verification was conducted of all of the components in the extracted vadose-zone module and the new pseudo-3D aquifer module in 2000. The modules were verified against analytical solutions and EPACMTP results.

EPACMTP and its predecessors have been validated using field data from four unique sites from 1990-1995. These sites include: the Borden site, the Long Island site, the Dodge City site, and the EBOS site 24.

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SUBAPPENDIX D.A

VADOSE-ZONE MODULE VERIFICATION RESULTS

(1993-1994)

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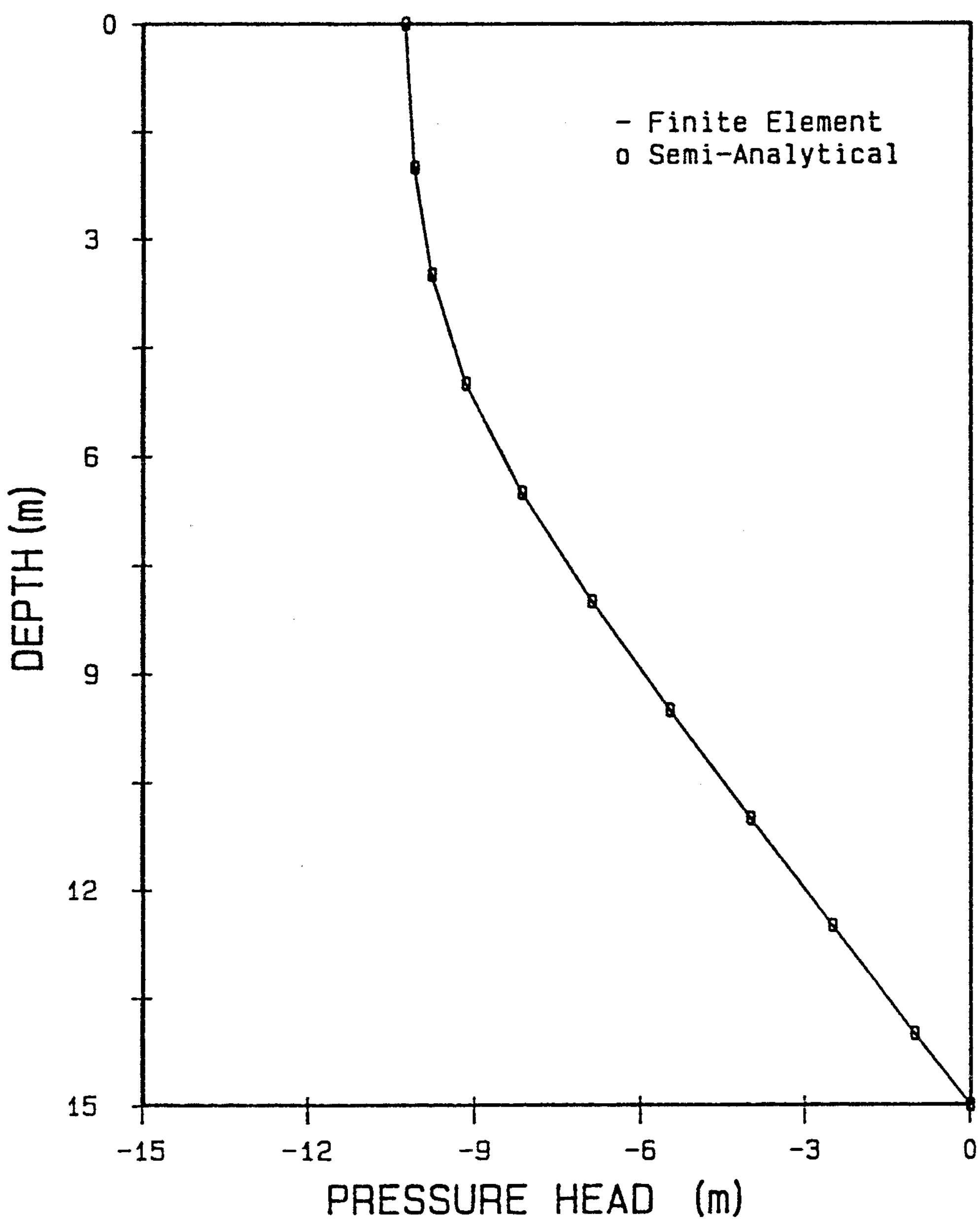


Figure D.A.1 Test Case 1: Predicted Pressure Head Distribution in the Unsaturated Zone. The Solid Line Represents Finite Element Solution, and Data Points Represent Semi-analytical Solution

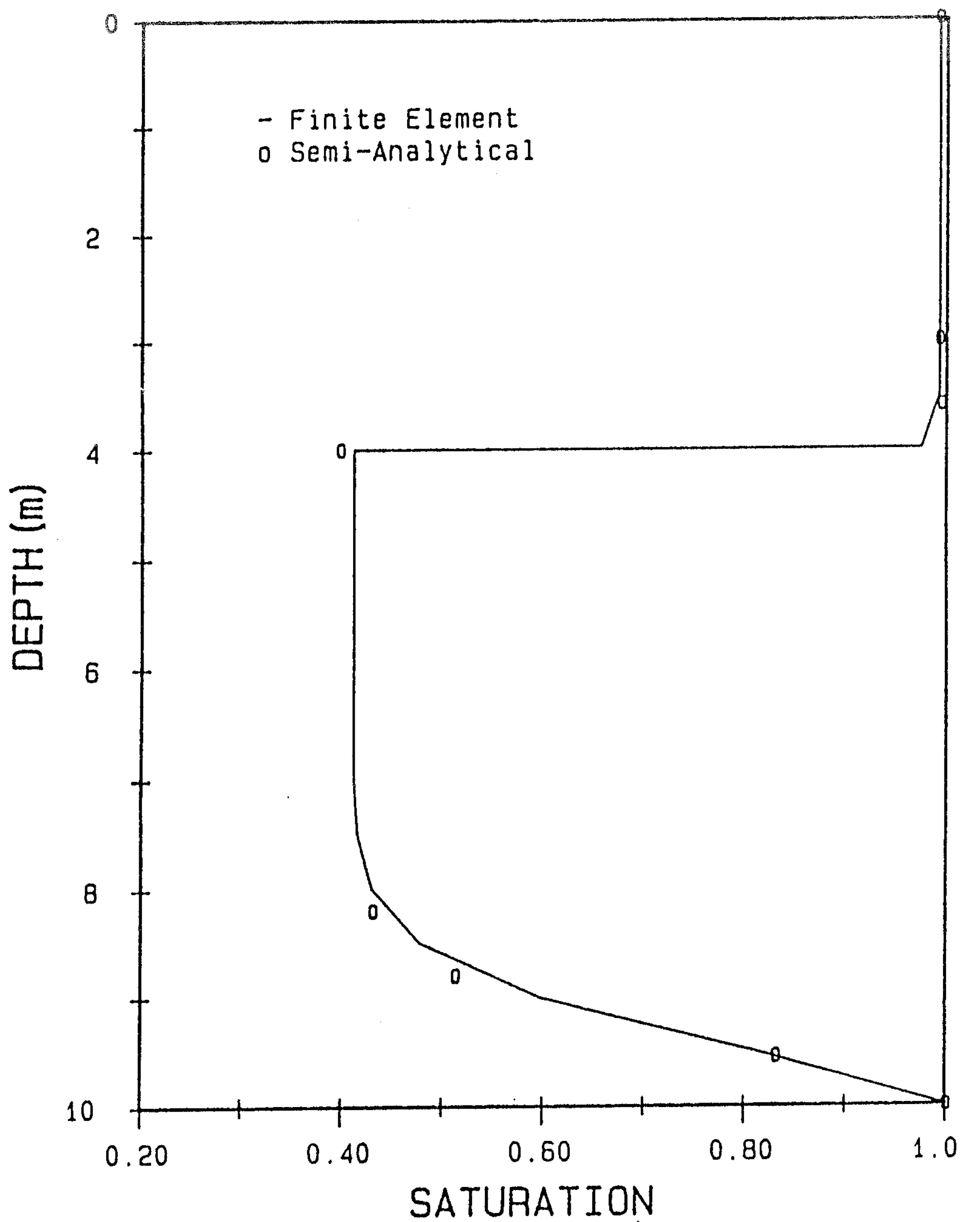


Figure D.A.2 Test Case 2: Predicted Saturation Distribution in the Unsaturated Zone. The Solid Line Represents the Finite Element Solution, Data Points Represent the Semi-analytical Solution

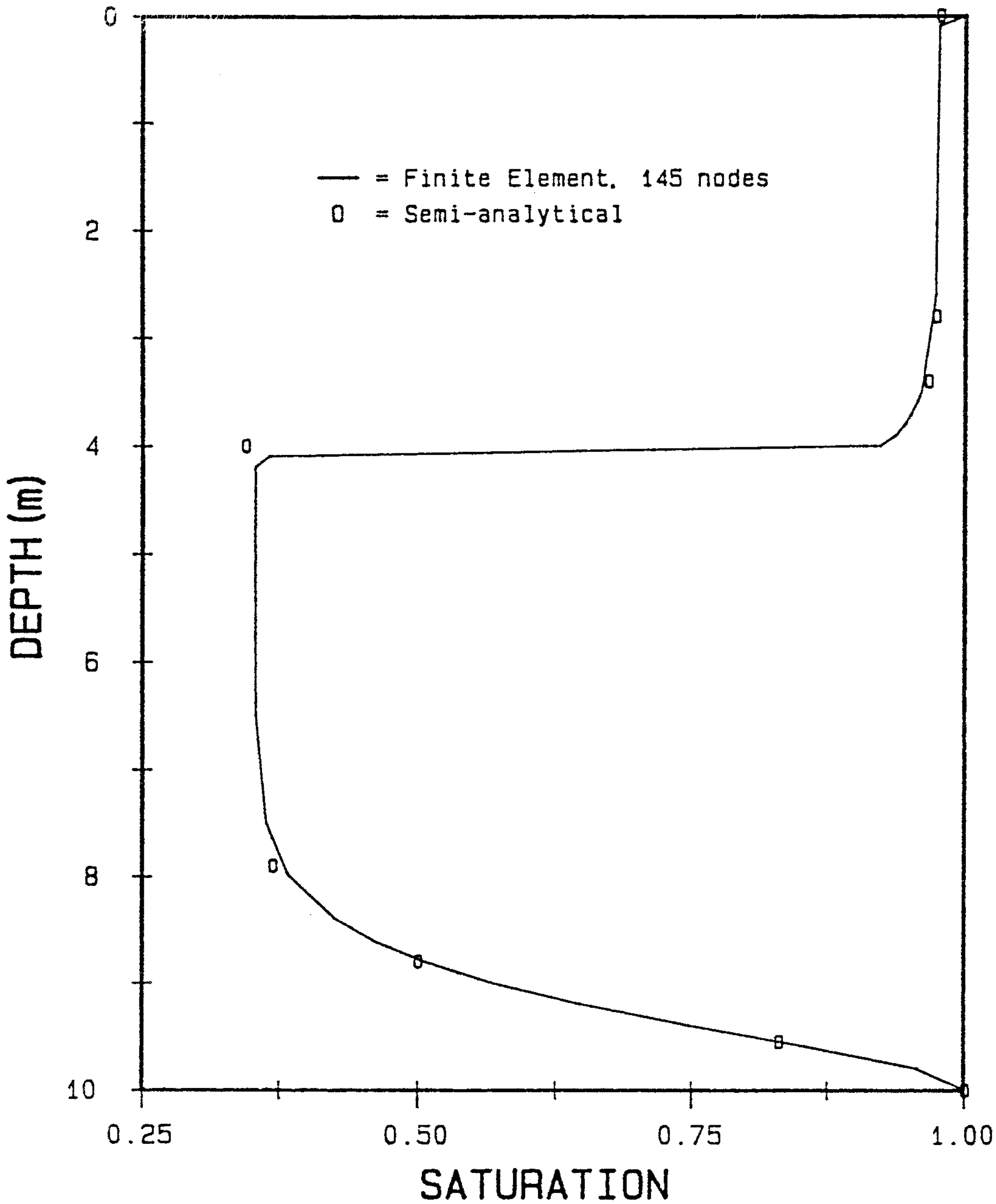


Figure D.A.3 Test Case 3: Predicted Saturation Distribution in the Unsaturated Zone. The Solid Line Represents the Finite Element Solution, and Data Points Represent the Semi-analytical Flow Solution

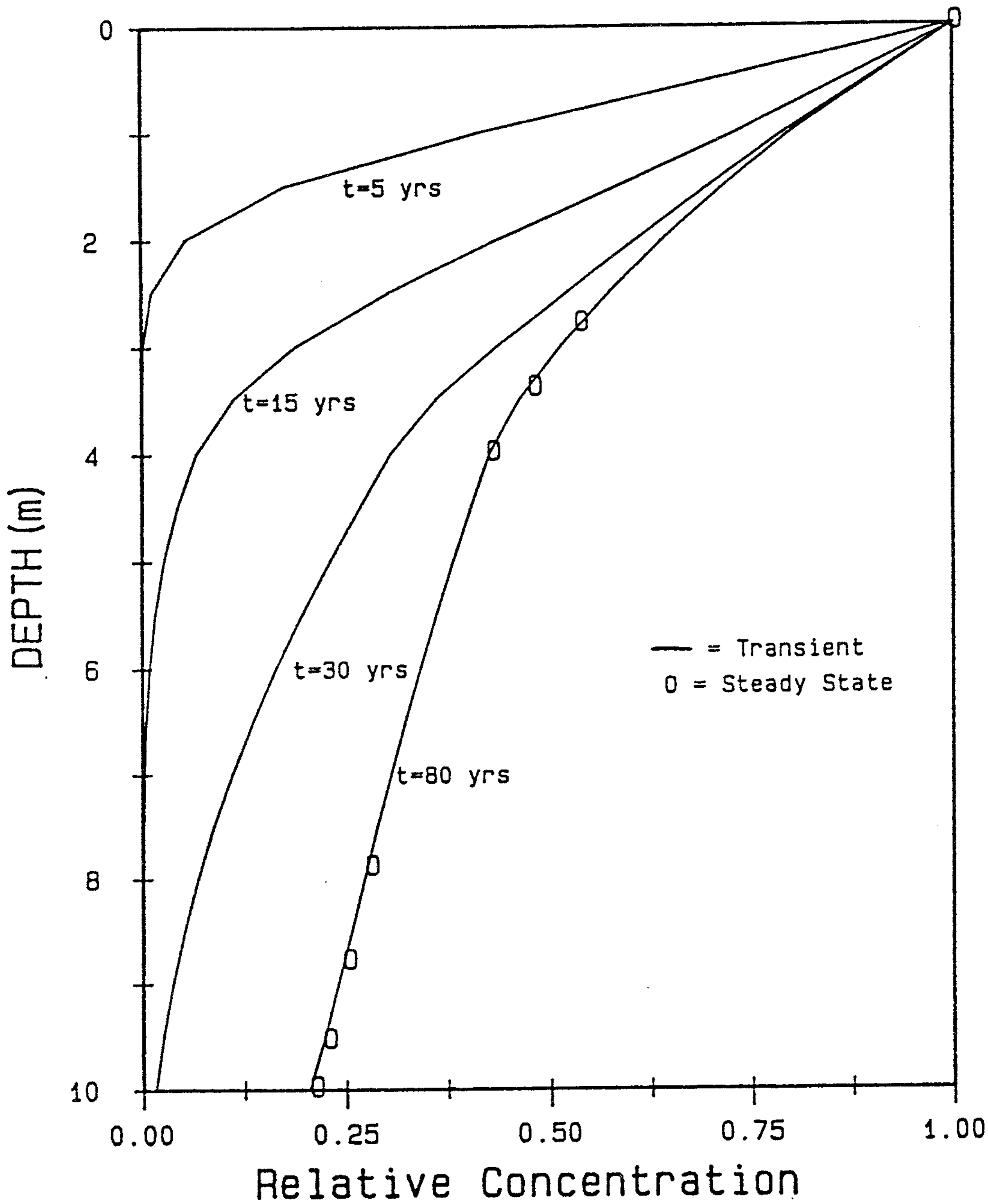


Figure D.A.4 Test Case 4: Transport in Layered Soil. The Solid Lines Correspond to the Transient Solution, Evaluated at t=5, 15, 30, and 80 Years. Data Points Represent the Steady-state Solution

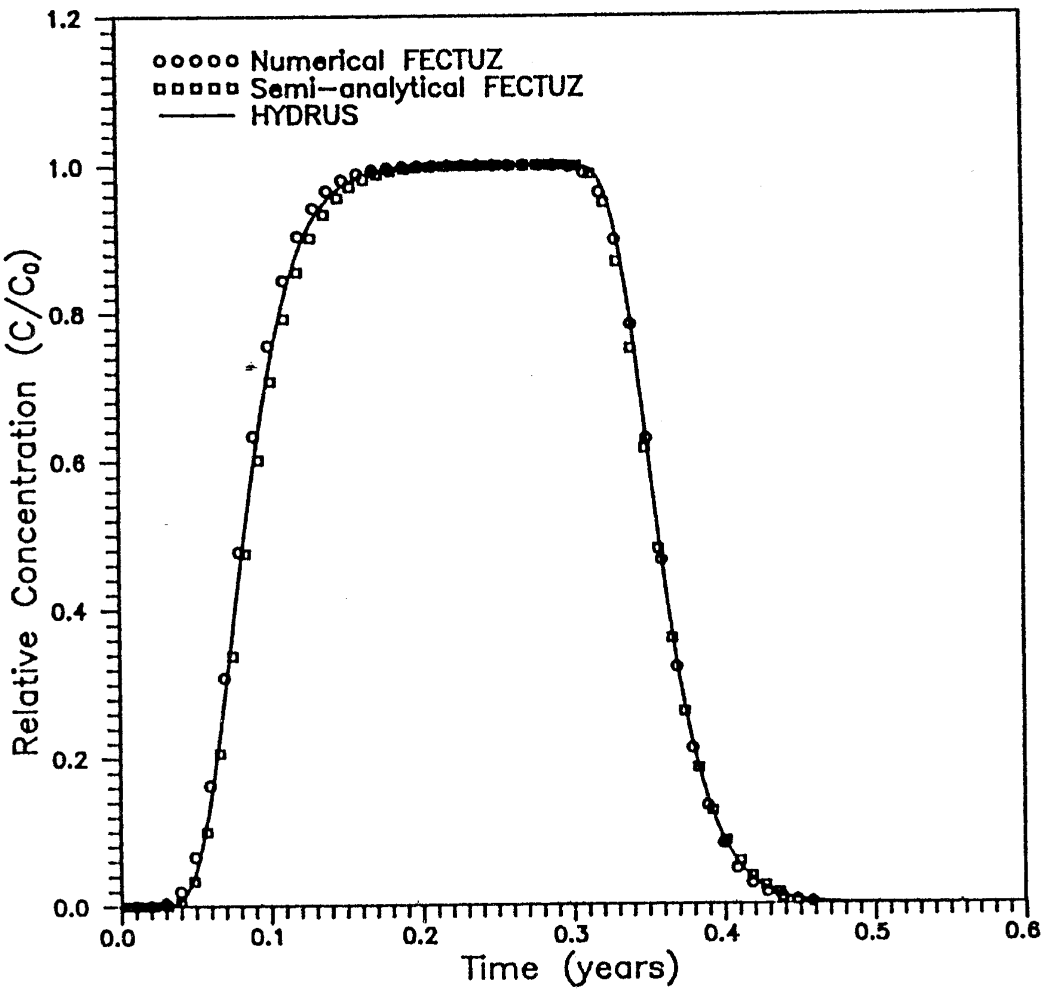


Figure D.A.5 Test Case 5: Comparison of Breakthrough Curves for the Transient Pulse Input Transport Problem. The Solid Line Represents the Solution of the Numerical HYDRUS Code, and the Data Points Represent the Semi-analytical and Numerical Transport Solution of FECTUZ

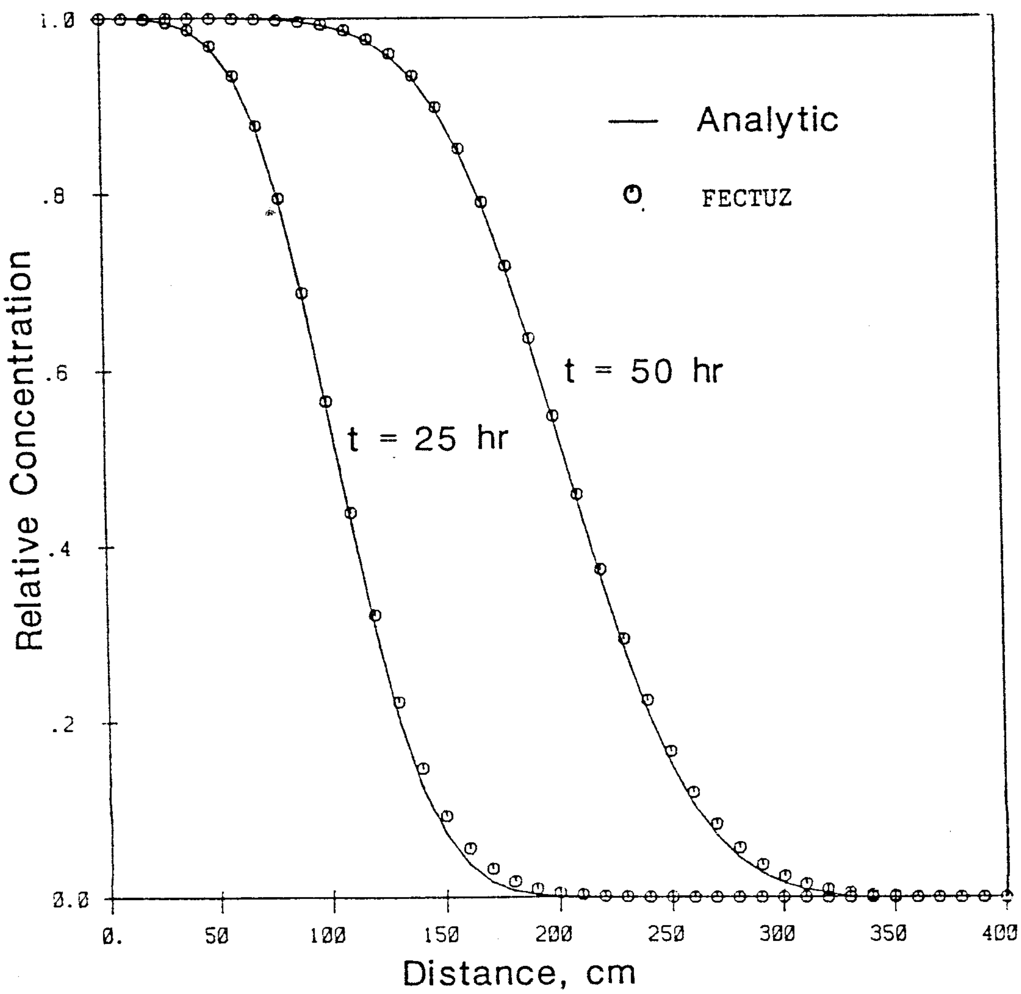
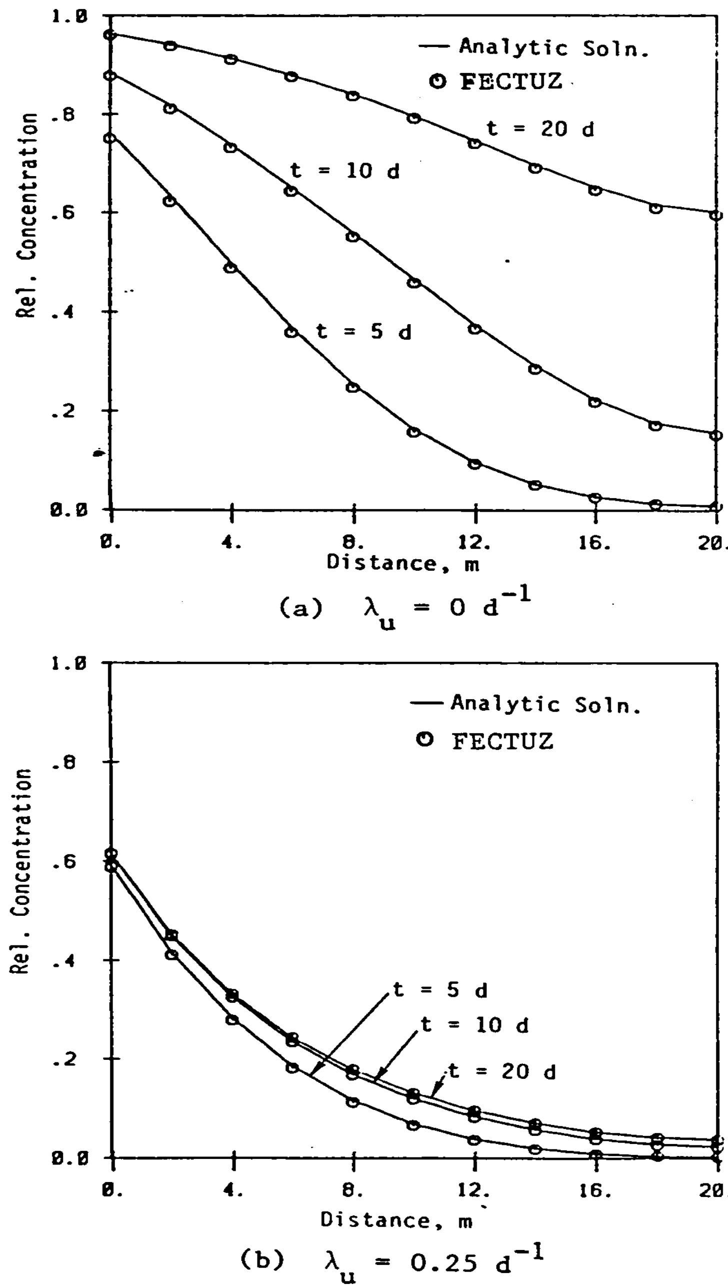


Figure D.A.6 Test Case 6: Simulated Concentration Profiles of Solute Transport in a Semi-infinite Soil Column. Solid Lines Represent the Analytical Solution. Data Points Represent the Numerical Solution of FECTUZ



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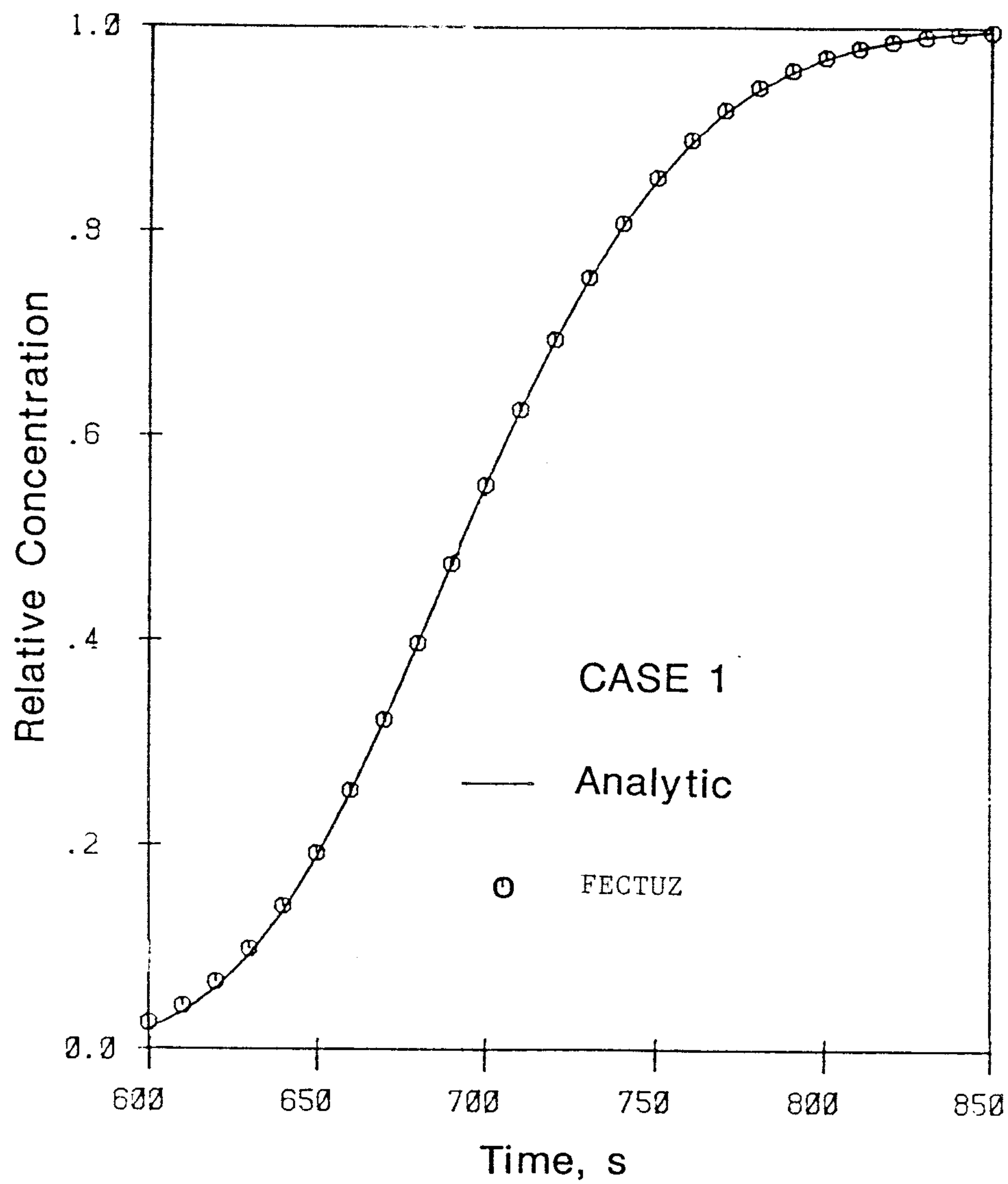


Figure D.A.8 Test Case 8, Sub-case 1: Simulated Outflow Breakthrough Curve of the Problem of Solute Transport in a Layered Soil Column. The Dispersivity Values Are 0.076 cm, 0.174 cm, and 0.436 cm for Layers 1, 2, and 3, Respectively. The Solid Line Represents the Analytical Solution While the Data Points Represent the Numerical Solution of FECTUZ

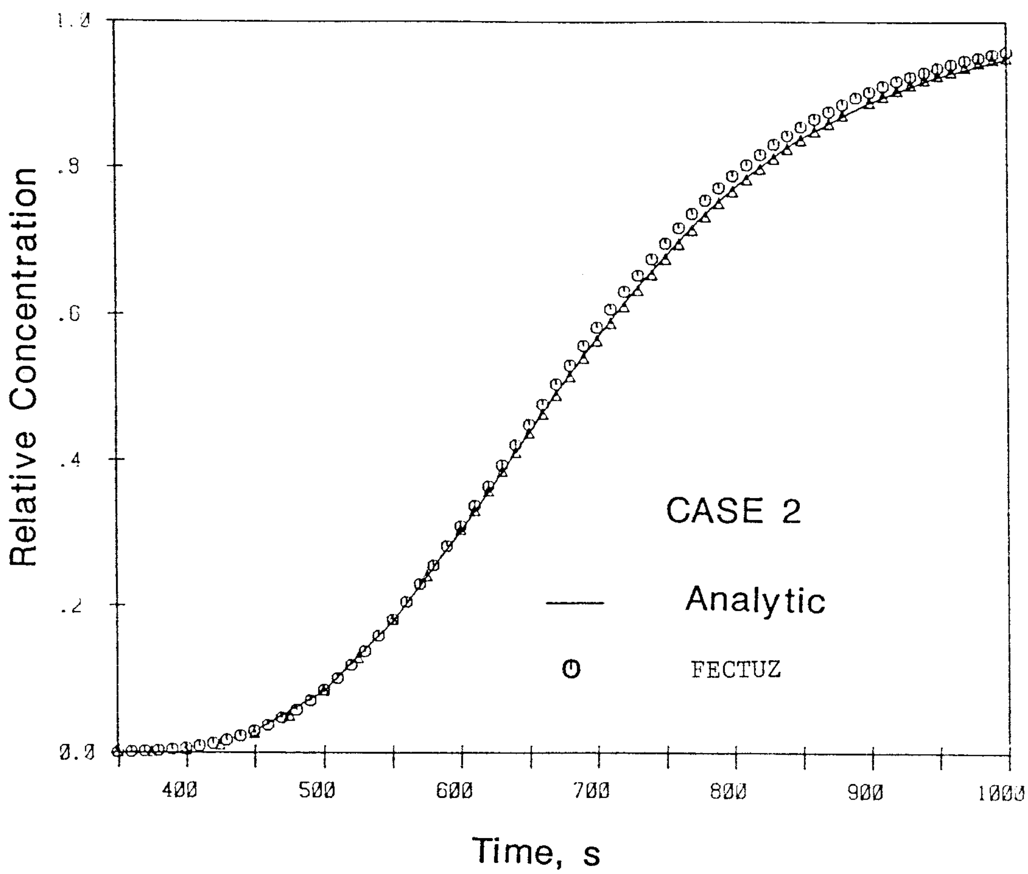


Figure D.A.9 Test Case 8, Sub-case 2: Simulated Outflow Breakthrough Curve of the Problem of Solute Transport in a Layered Soil Column. The Dispersivity Values Are 0.76 cm, 1.74 cm, and 4.36 cm for Layers 1, 2, and 3, Respectively. The Solid Line Represents the Analytical Solution While the Data Points Represent the Numerical Solution of FECTUZ

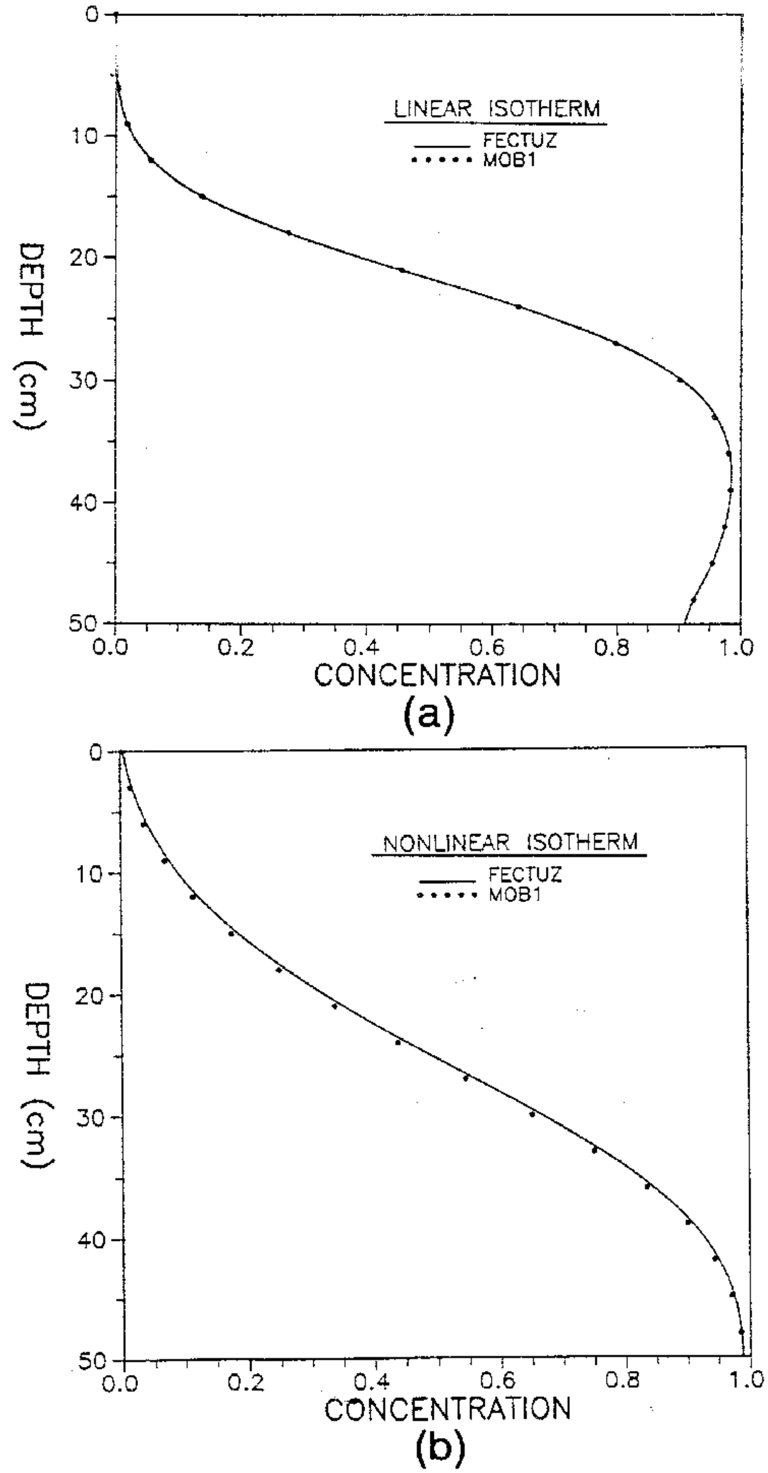
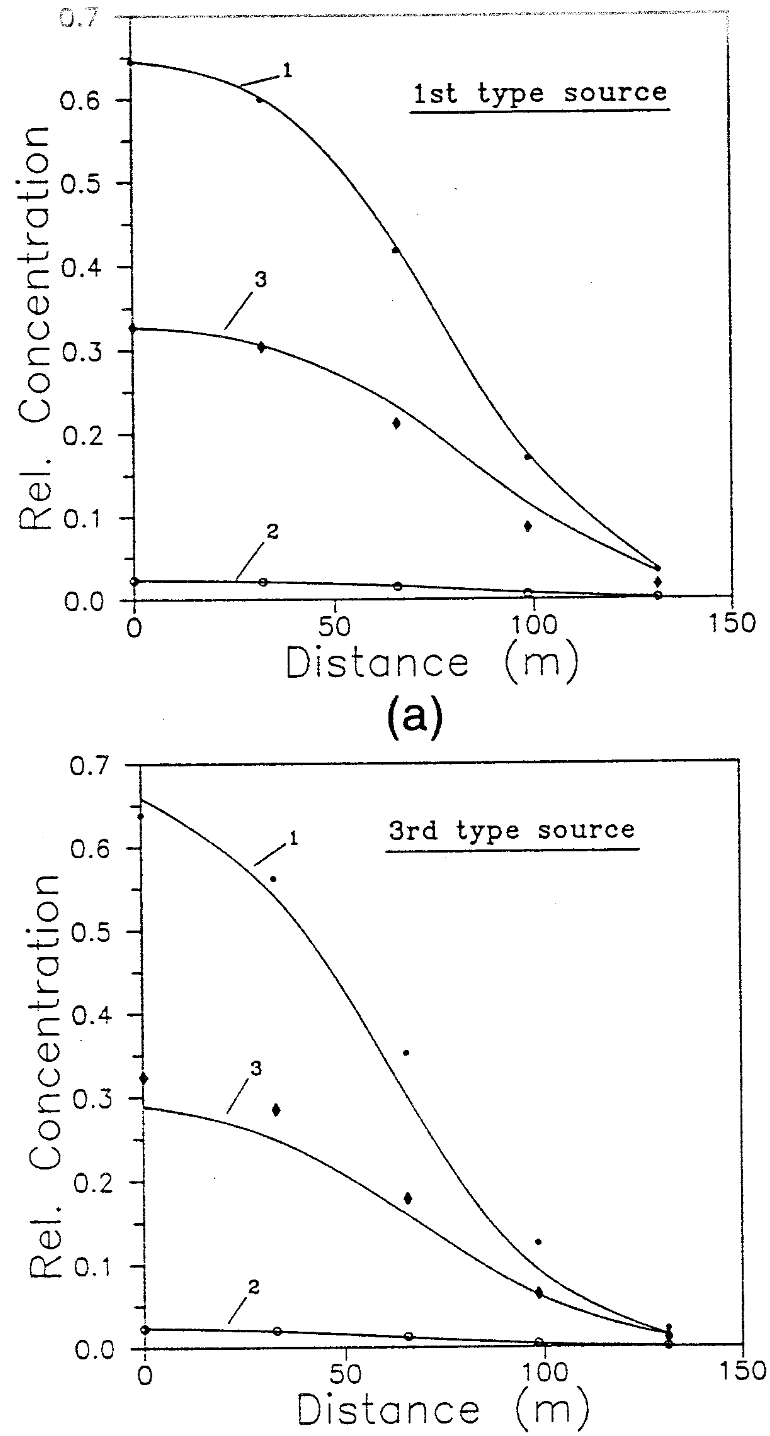


Figure D.A.10 Test Case 9: Comparison Between FECTUZ and MOB1 for Test Case 9, (a) Linear Adsorption and (b) Nonlinear Adsorption. The Solid Line Represents the Finite Element Solution of FECTUZ While the Data Points Represent the Finite Difference Solution of MOB1



(a)

(b)

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SUBAPPENDIX D.B

AQUIFER-MODULE VERIFICATION RESULTS (1993-1994)

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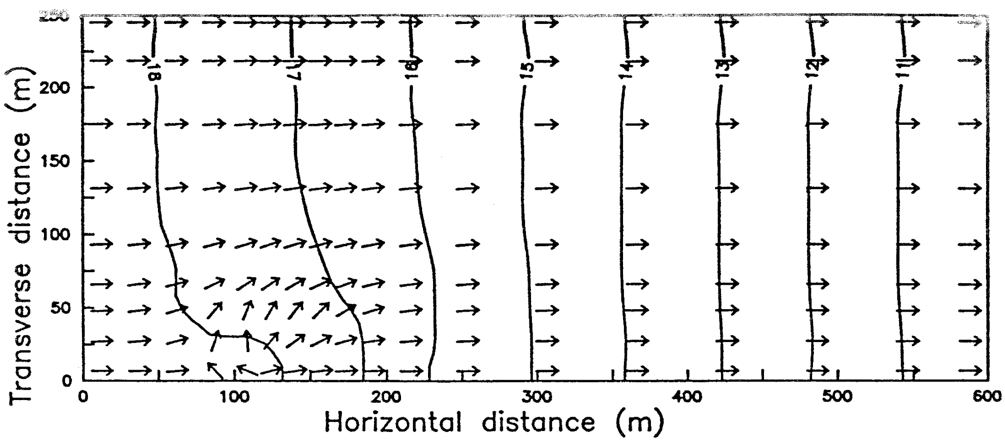
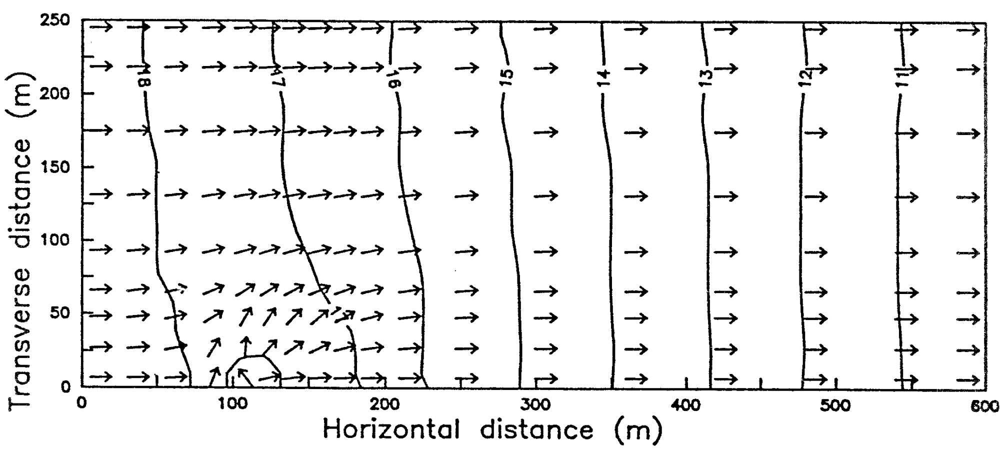


(A)



(B)

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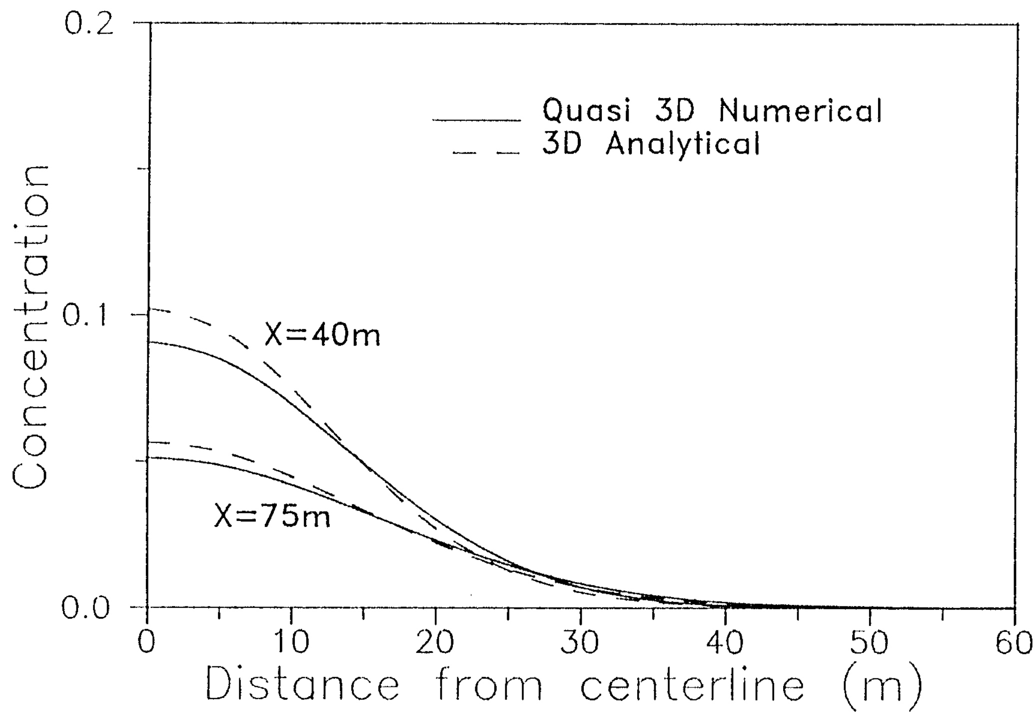


Figure D.B.2 Test Case 2: Comparison of Predicted Horizontal Transverse Concentration Profiles at X=40 M and X=75 M from the Source

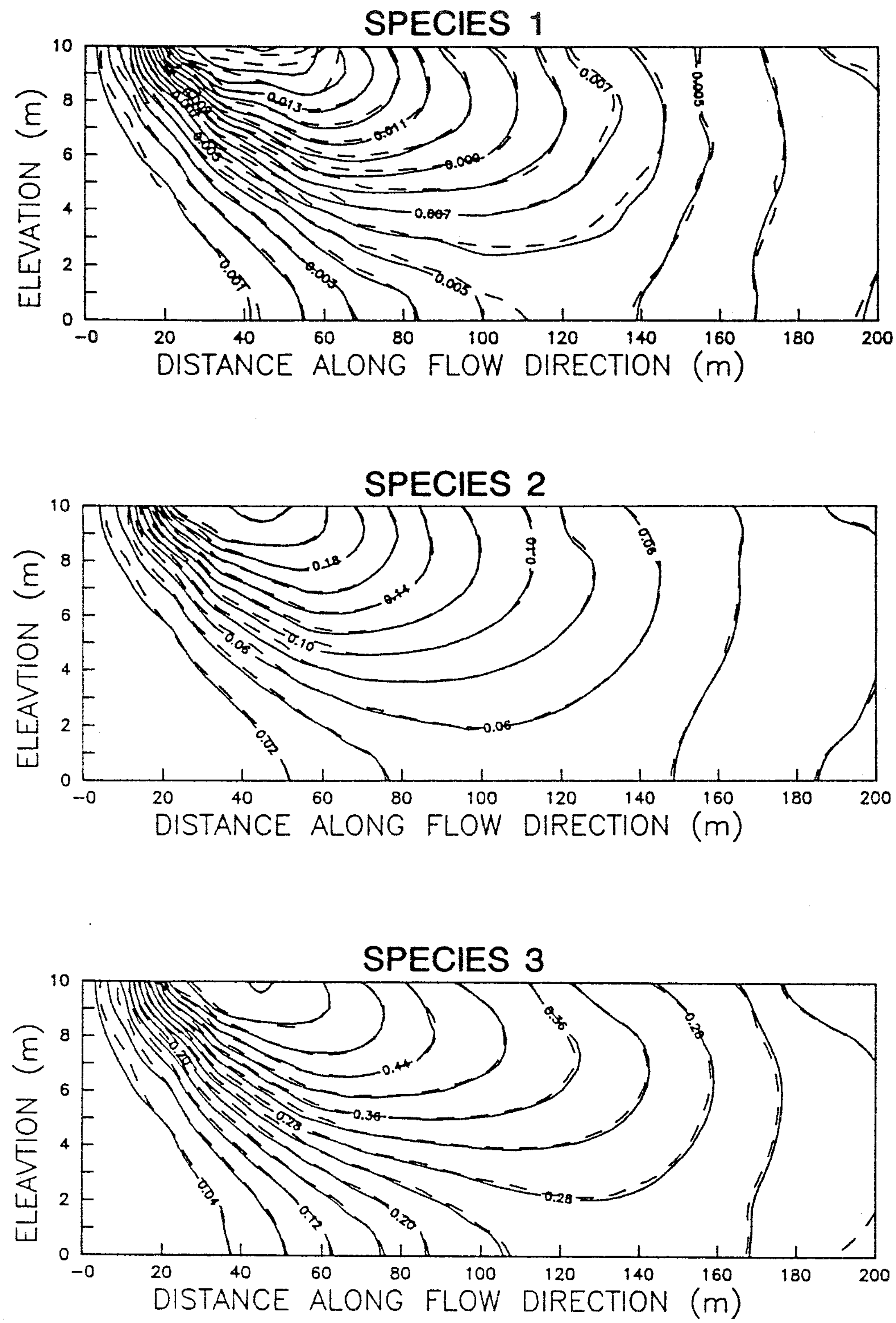
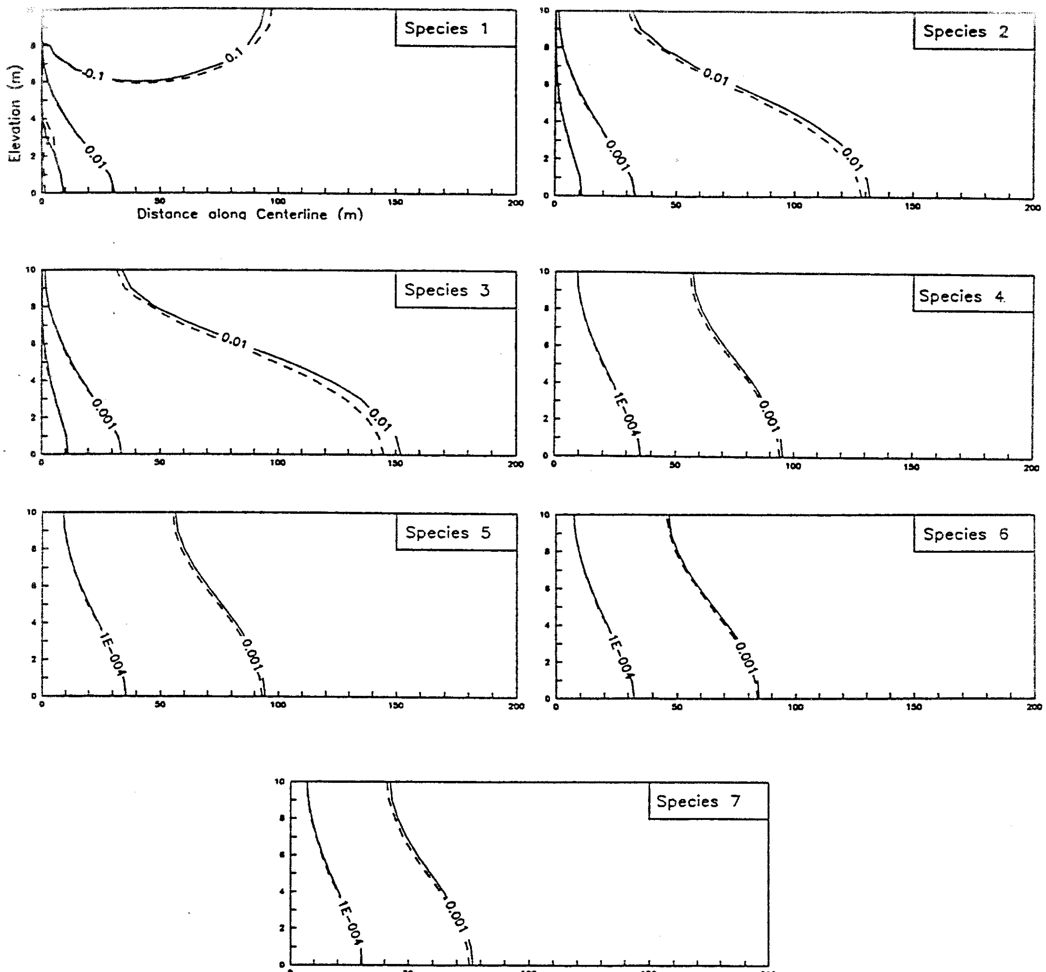


Figure D.B.3 Test Case 3: Comparison of CANSAZ-3D (Solid Contours) and VAM2D (Dashed Contours)



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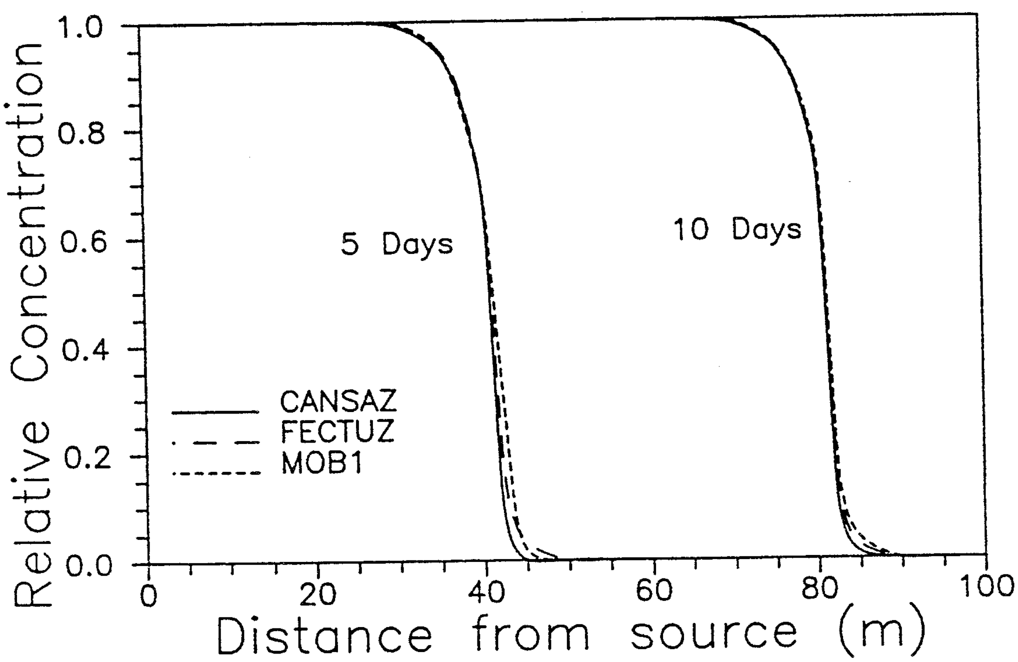

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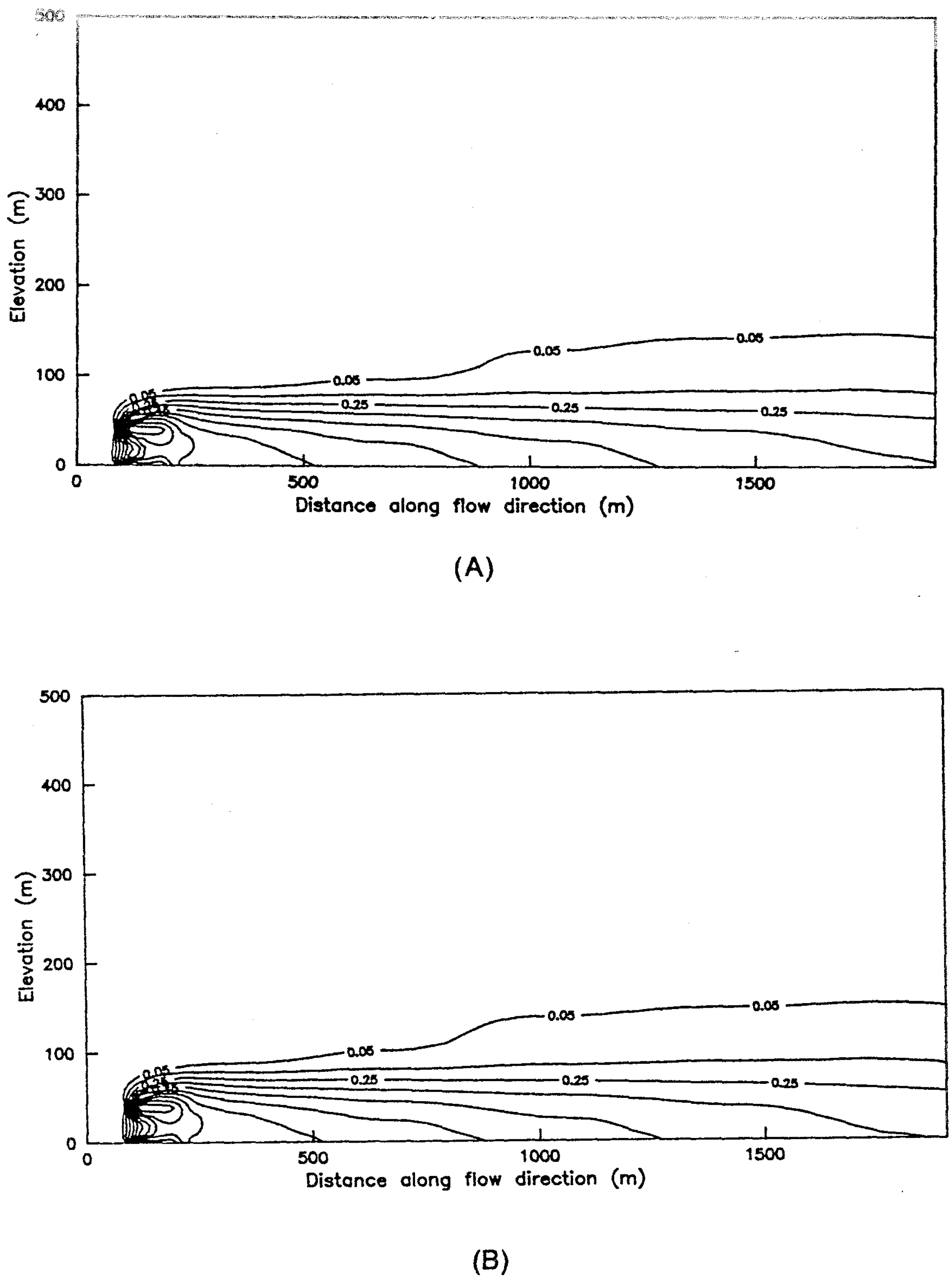

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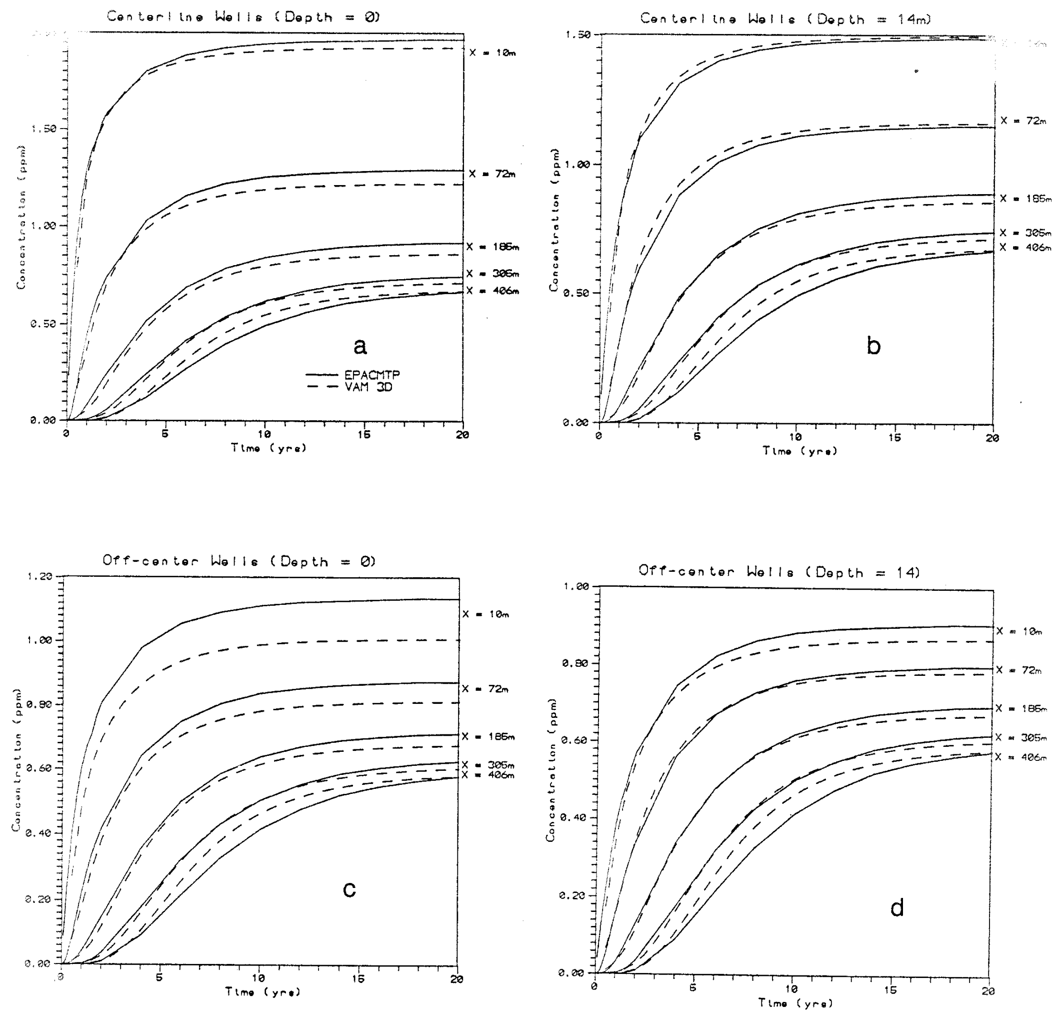

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SUBAPPENDIX D.C

RESULTS (1993-1994)

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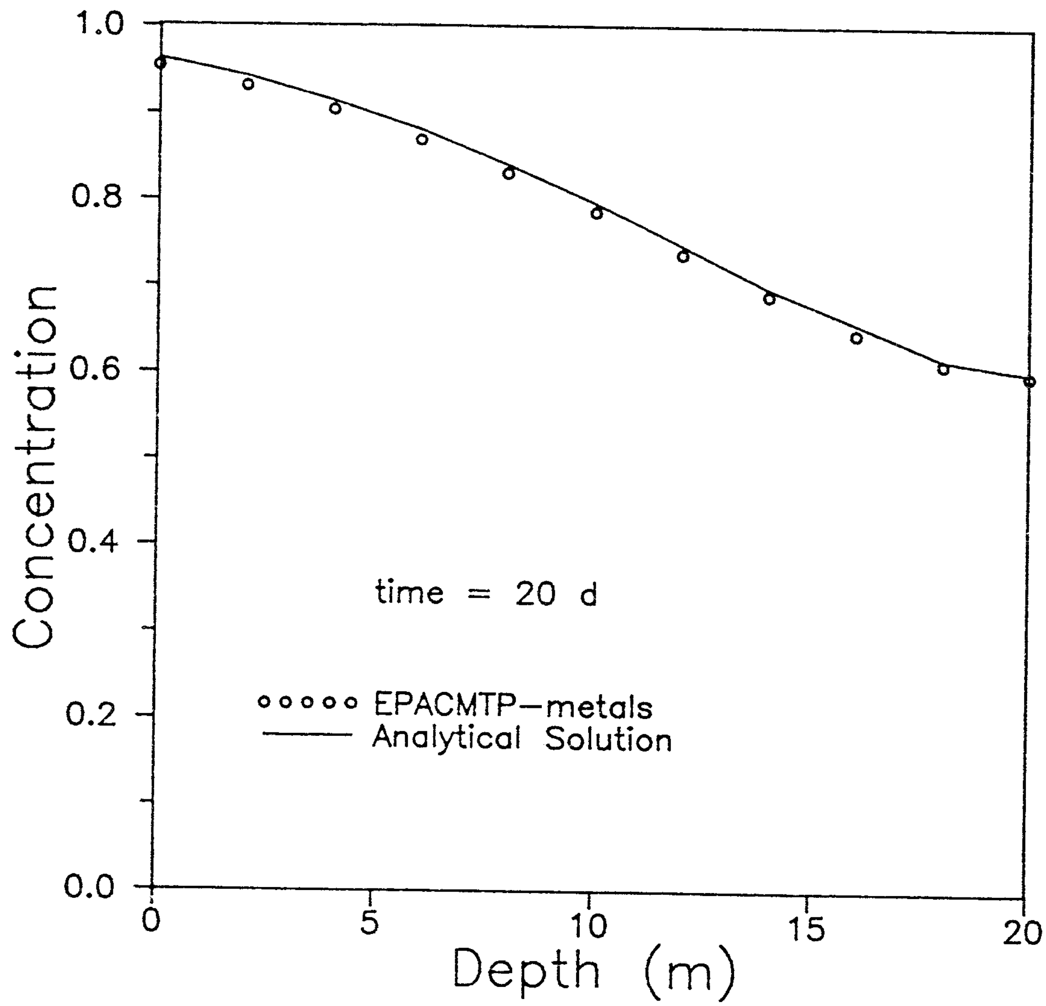

Figure D.C.1 Test Case 1: Comparison of EPACMTP-Metals Result with Analytical Solution for the Unsaturated-zone with Linear Adsorption Isotherm

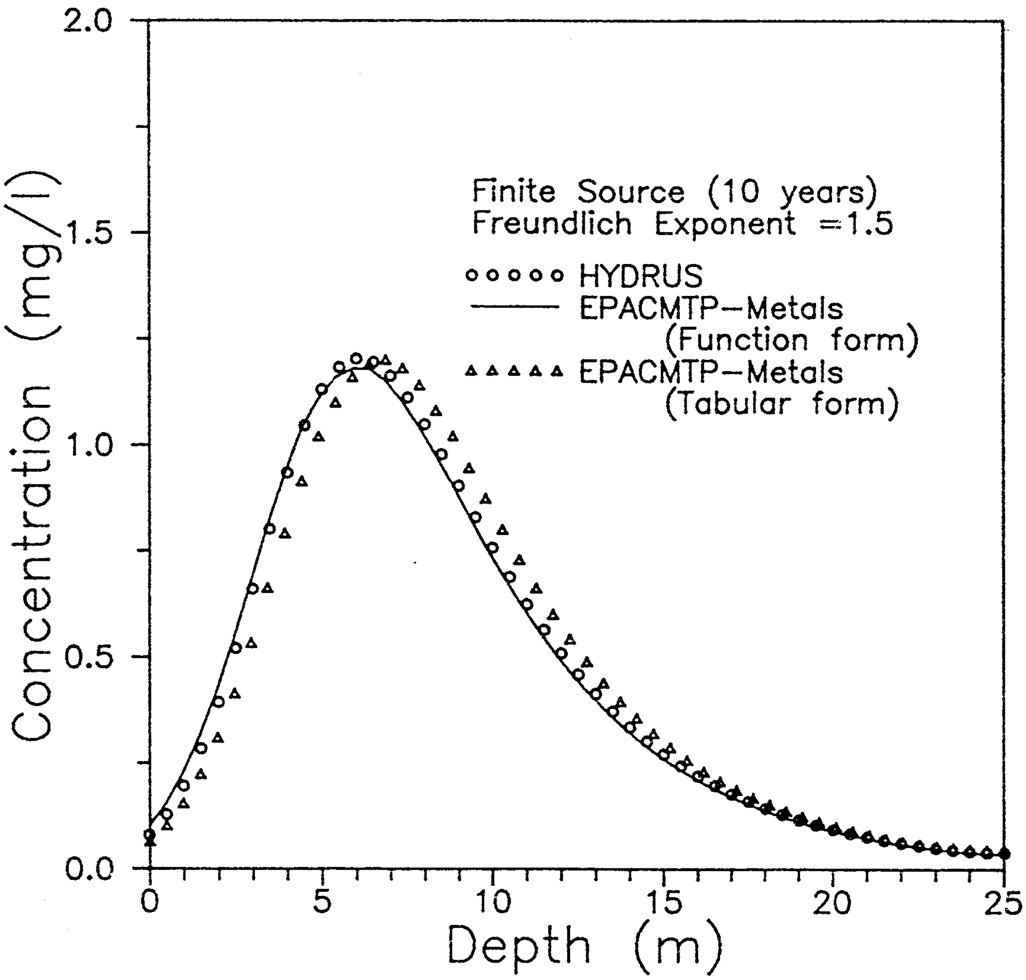

Figure D.C.2 Test Case 2, Finite Source: Comparison of Unsaturated Zone Concentration Profiles of HYDRUS and EPACMTP-Metals for Nonlinear Adsorption with Freundlich Exponent = 1.5

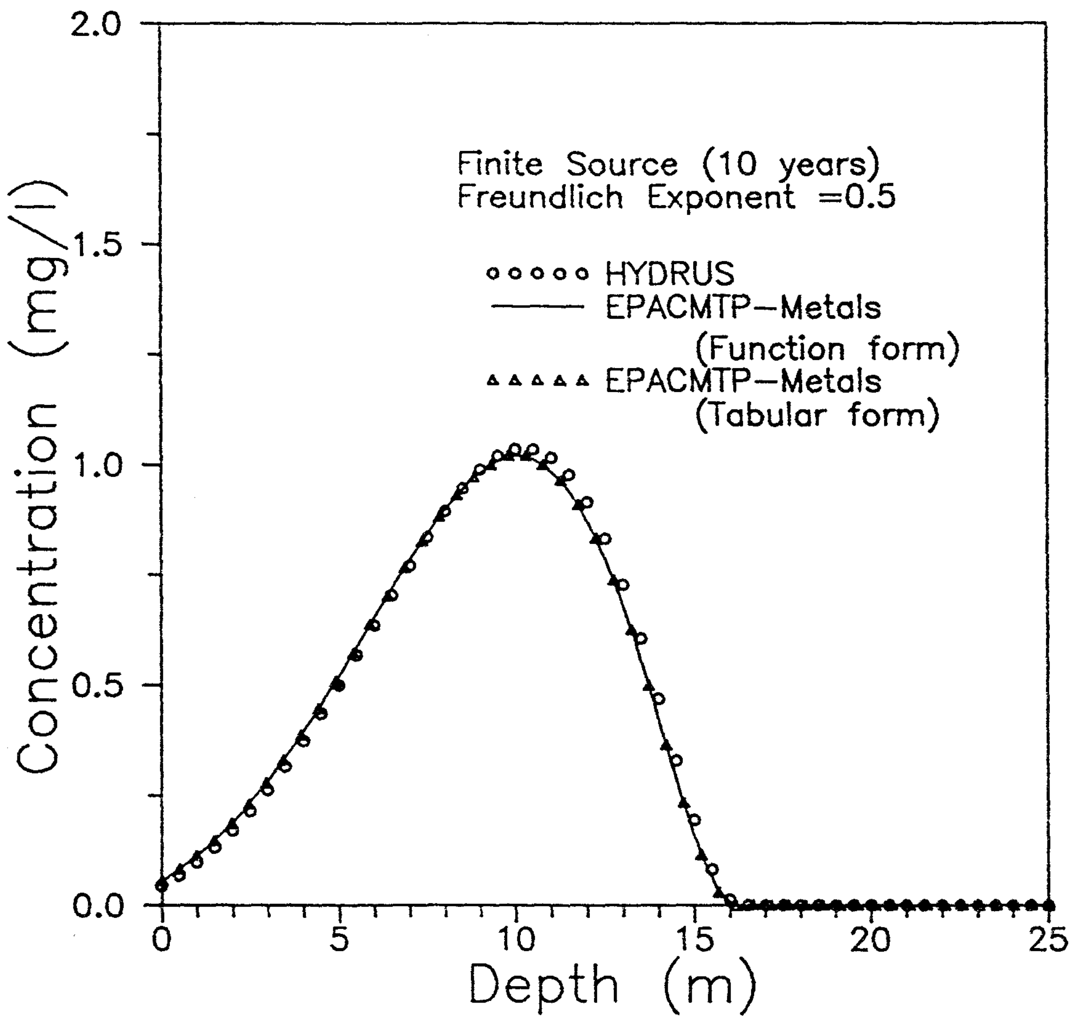

Figure D.C.3 Test Case 2, Finite Source: Comparison of Unsaturated Zone Concentration Profiles of HYDRUS and EPACMTP-Metals for Nonlinear Adsorption with Freundlich Exponent = 0.5

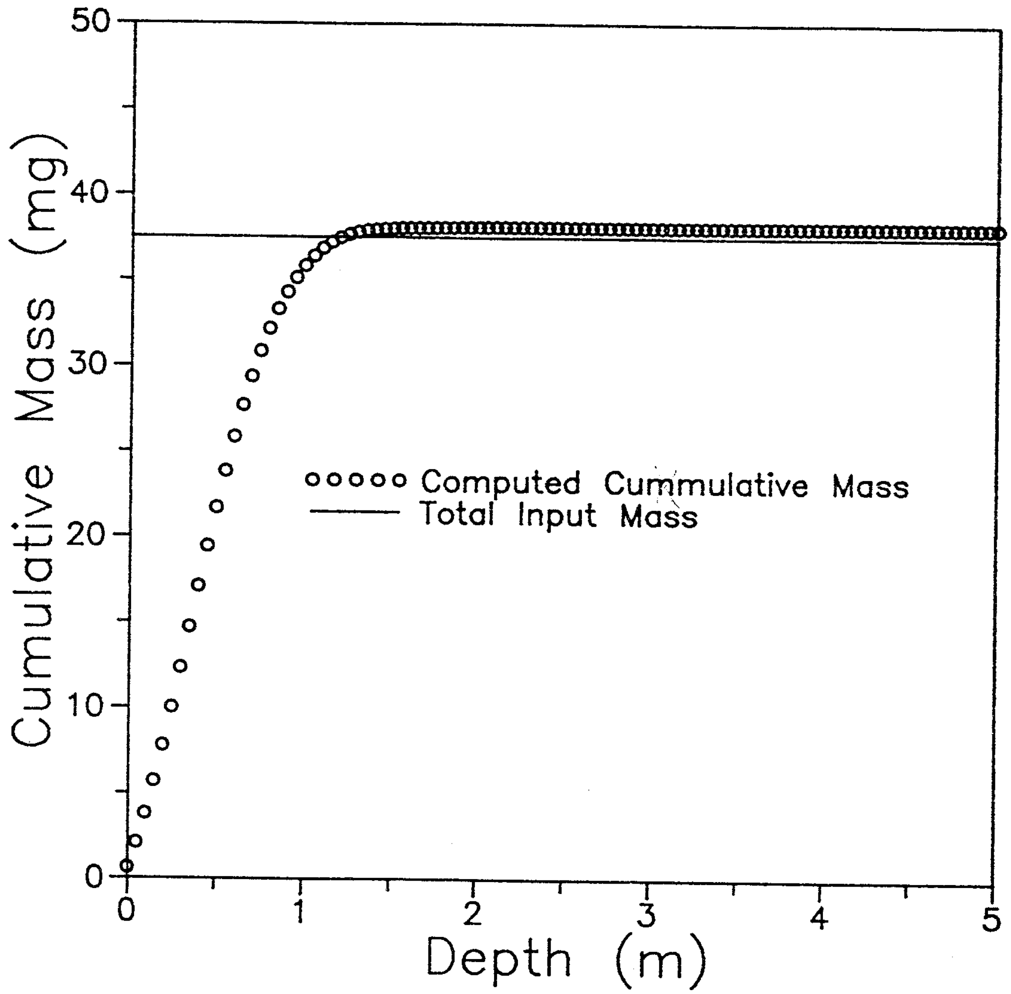

Figure D.C.4 Test Case 3: Cumulative Mass in the Unsaturated Zone and Total Input Mass for Lead Isotherm #3 Corresponding to Low Organic Acids (LOA), Low HFO, Low POM, and High pH Condition

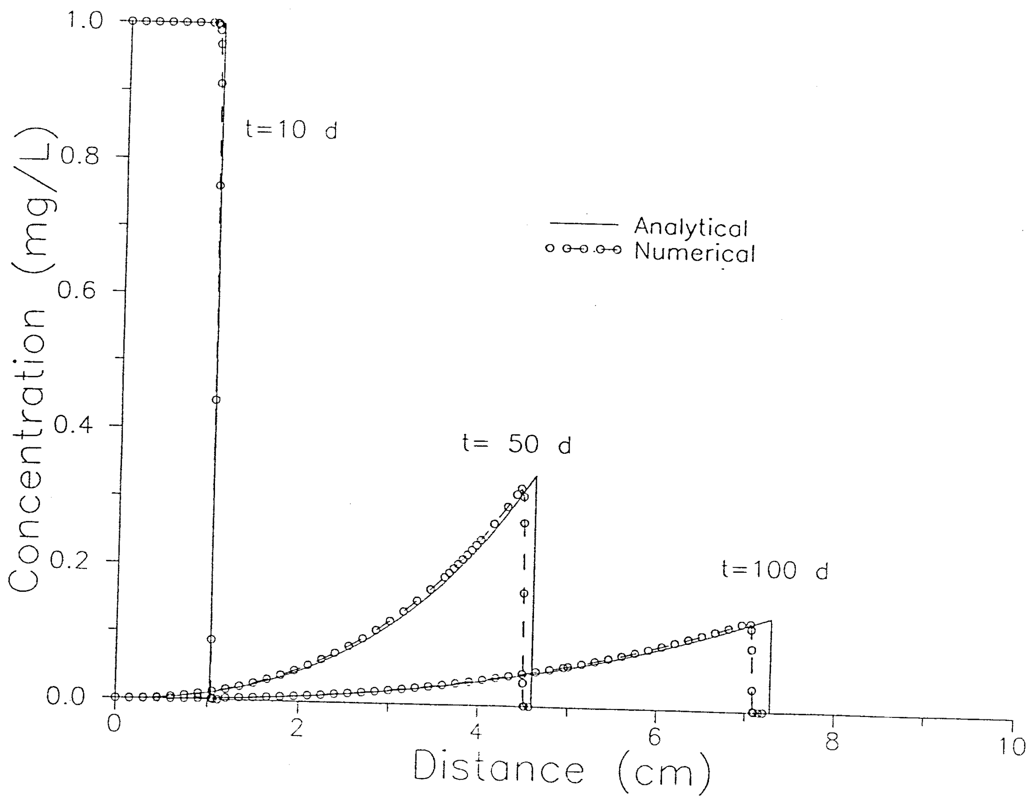

Figure D.C.5 Test Case 4: Comparison of Concentration Profiles for Freundlich Exponent = 0.5

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VADOSE-ZONE MODULE VERIFICATION RESULTS (1997)

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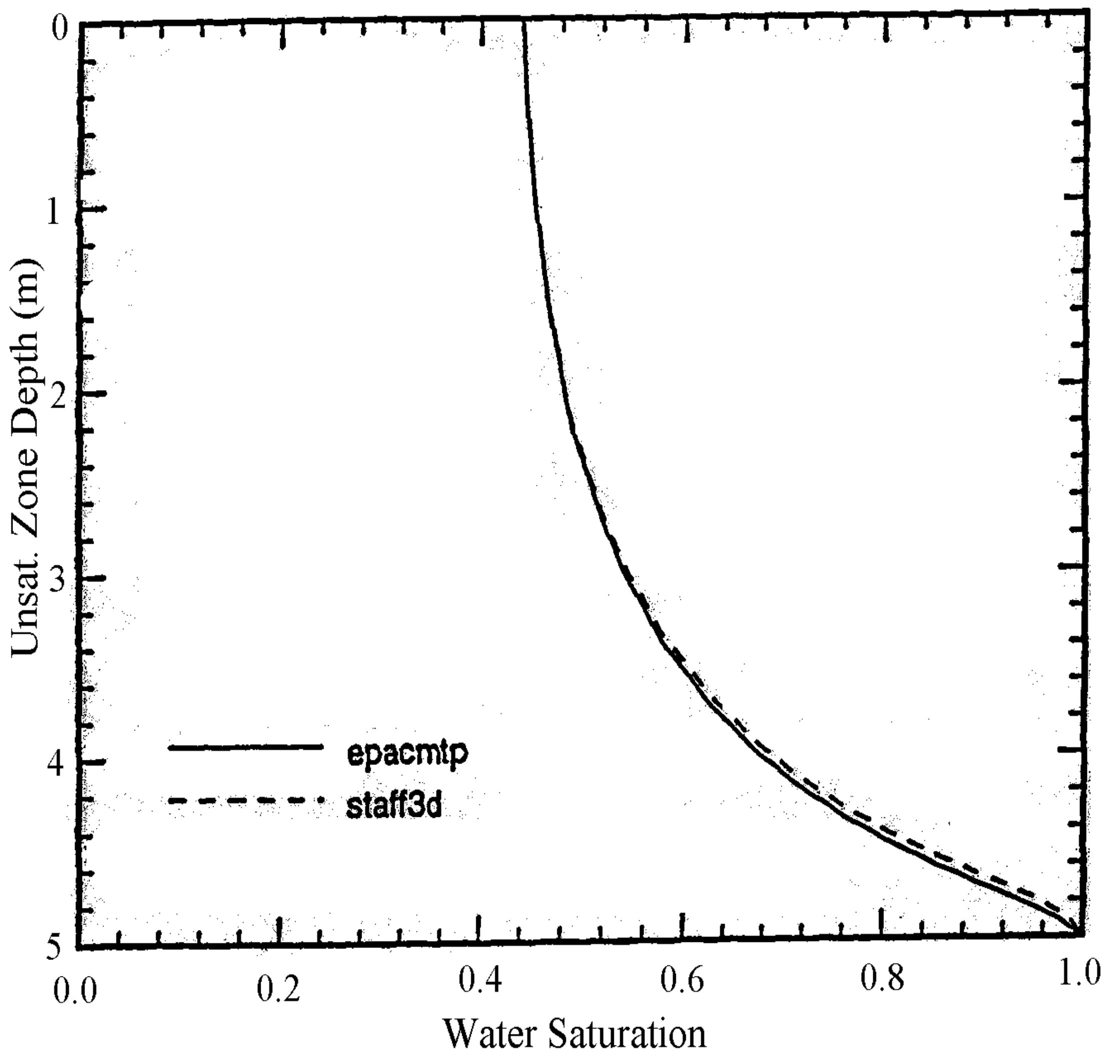

Figure D.D.1 Test Case 1: Soil Water Saturation Profile, as a Function of Elevation, Where the Water Table Is Located at 5 Meters and Source Infiltration Q_r = 0.5 M/y

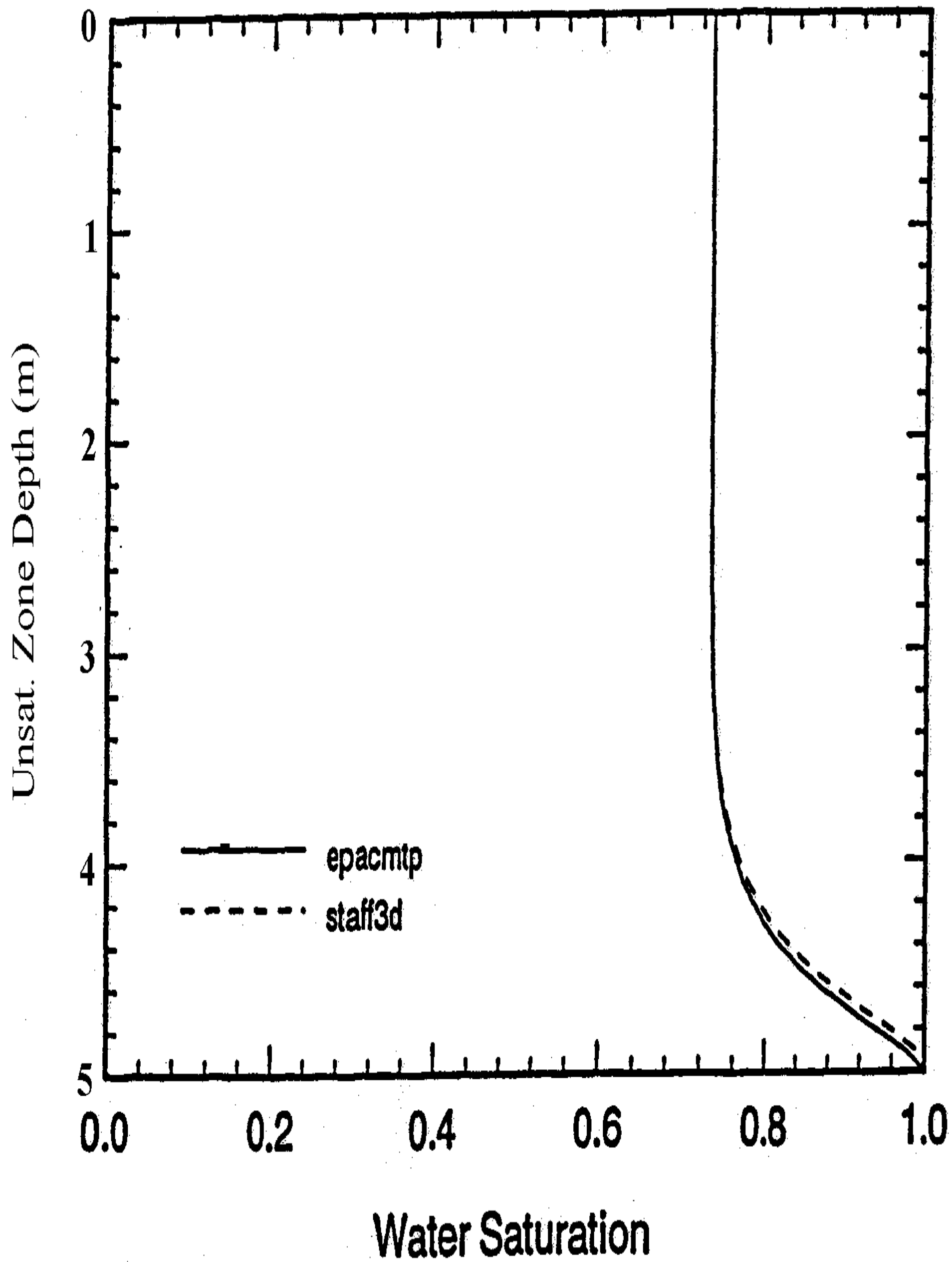

Figure D.D.2 Test Case 2: Soil Water Saturation Profile, as a Function of Unsaturated Zone Depth for a Surface Impoundment Scenario

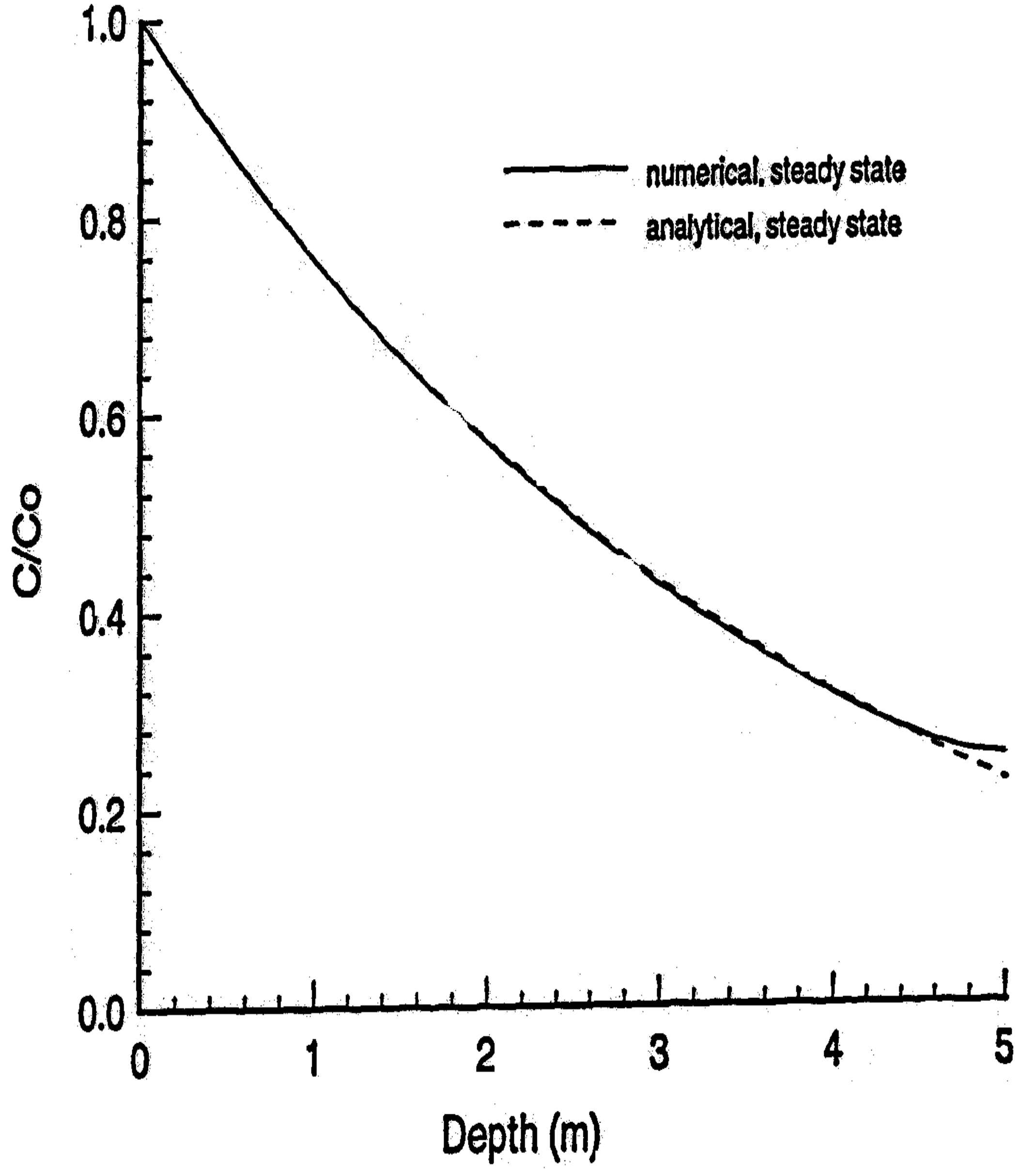

Figure D.D.3 Test Case 3: Steady-state Contaminant Concentration Profile, Where the Ground Surface Is Located at 0.0 M and the Water Table Is Located at 5.0 m

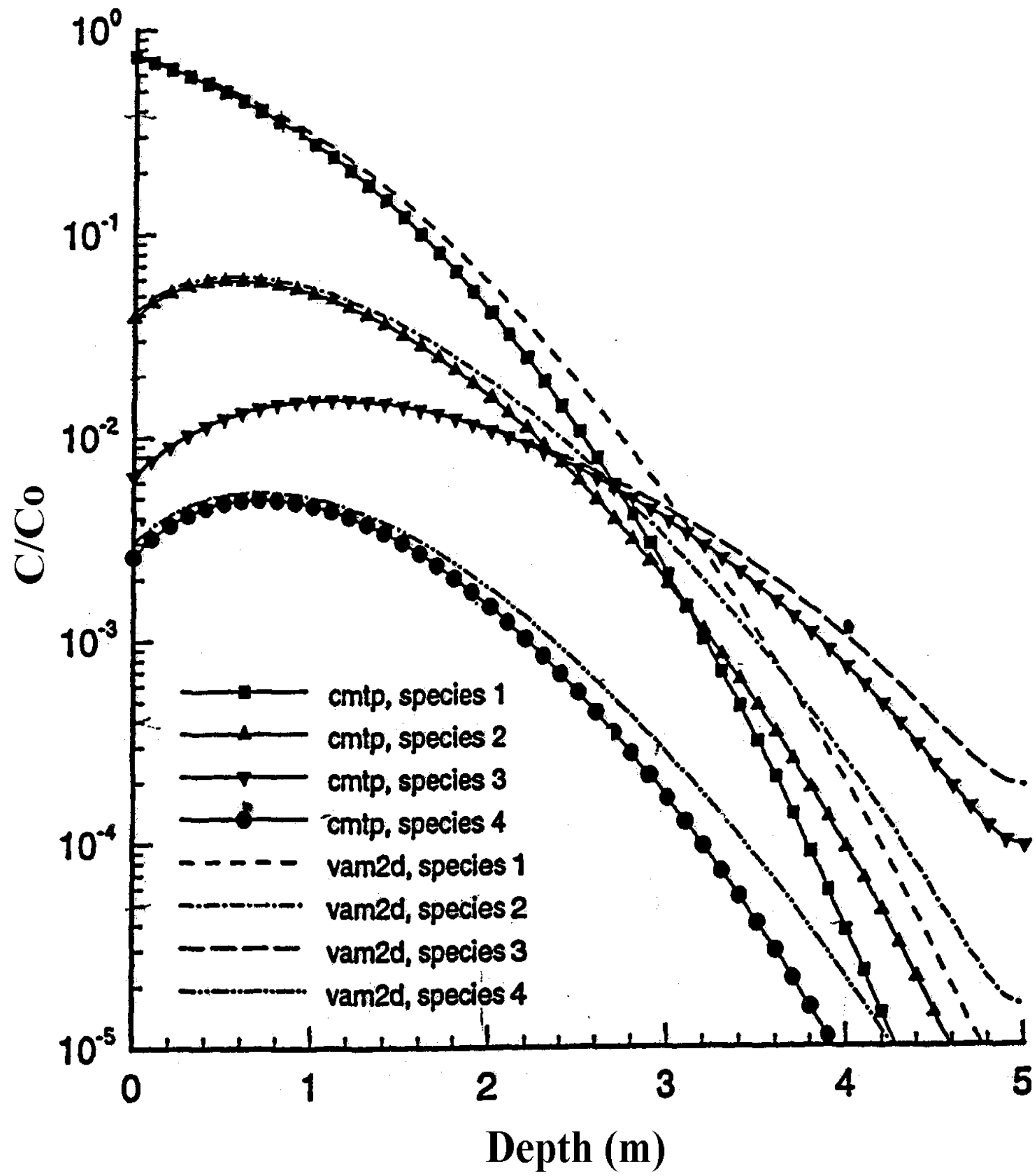

Figure D.D.4 Test Case 4: Contaminant Concentration Profiles as a Function of Depth for Four Species Involved in Branched Chain Decay at Time T=250 Days. The Ground Surface Is Located at 0.0 M and the Water Table Is Located at 5.0 m

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AQUIFER MODULE VERIFICATION RESULTS (1997)

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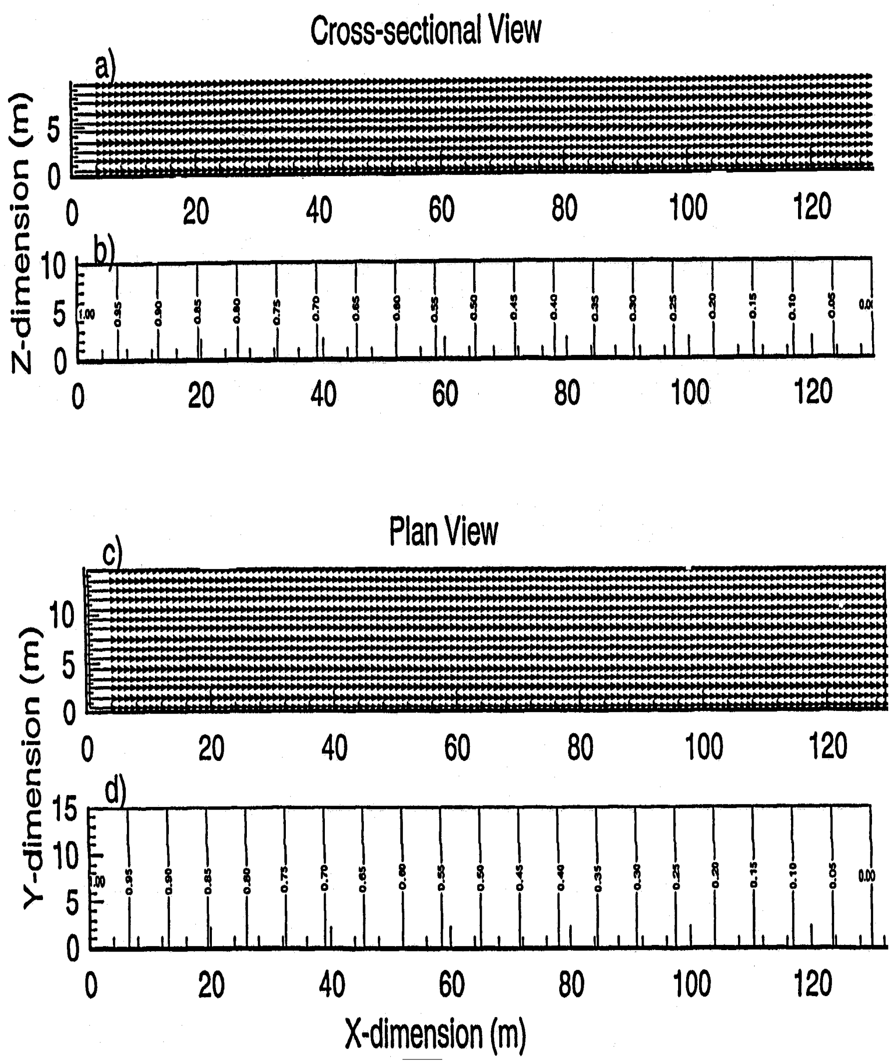
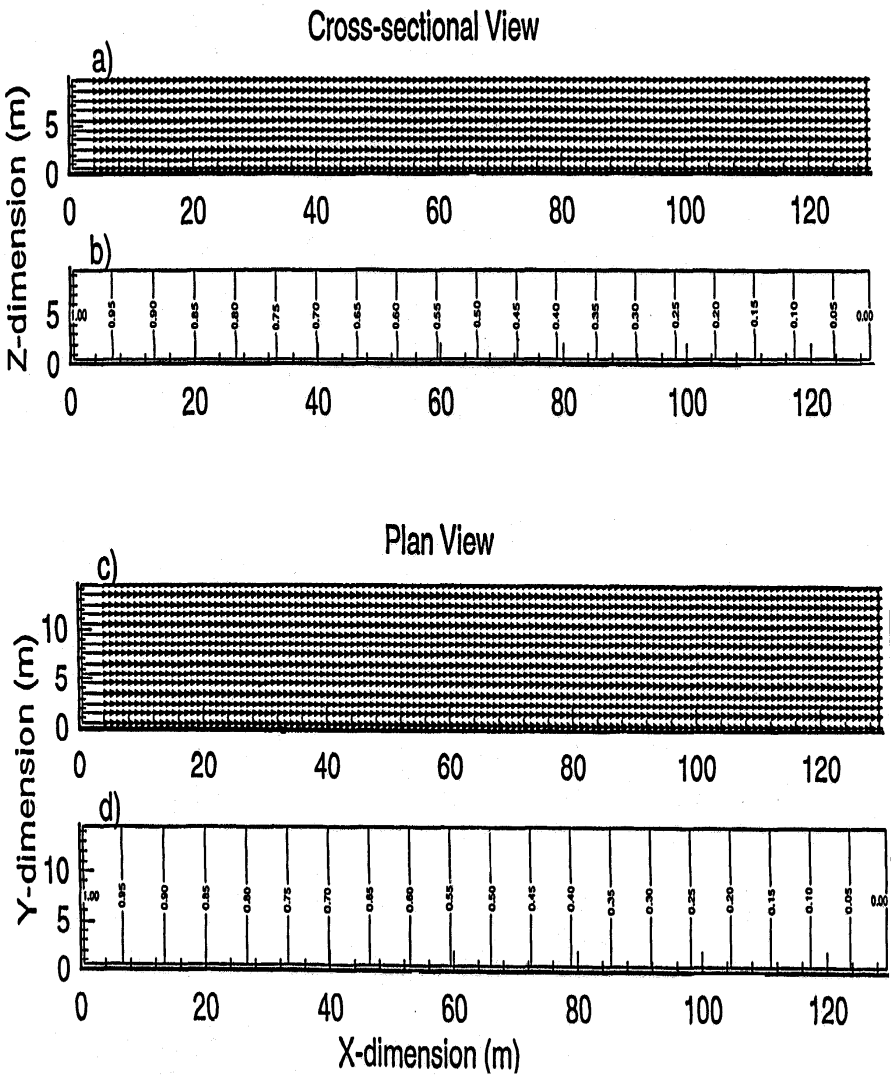


Figure D.E.1 Test Case 5: Steady State Groundwater Flow, Calculated by EPACMTP Distributions of Darcy Velocity Vectors (A) and Hydraulic Head (B) along the Vertical Cross-sectional Views (Z-x); Areal (X-y) Distributions of Darcy Velocity Vector (C) and Hydraulic Head (D) at the Top of the Saturated Zone



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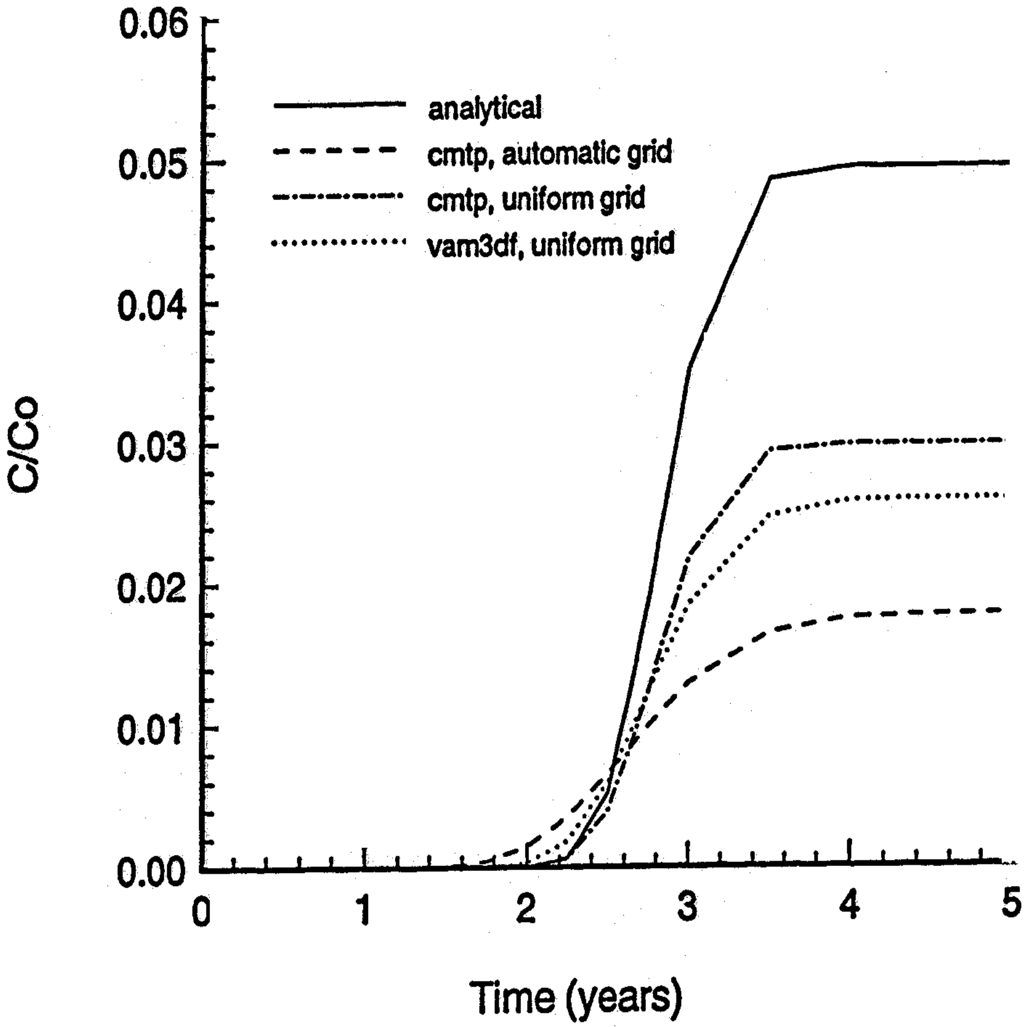
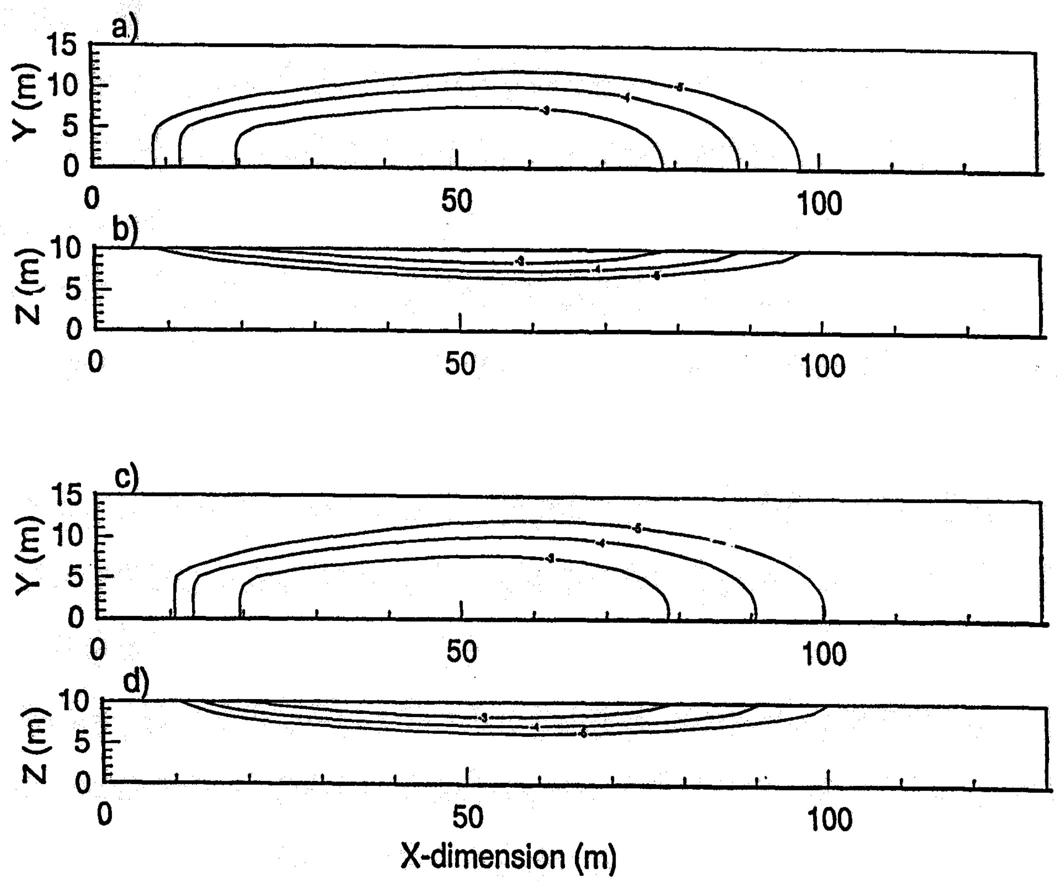


Figure D.E.3 Test Case 6: Concentrations Breakthrough Curves at a Receptor Well Located at the Top of Saturated Zone 100m Downgradient of the Source for Simulations Obtained with EPACMTP Analytical and Numerical (Automatic and Uniform Grid) Solutions and VAM3DF Solution (Uniform Grid)



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COMPOSITE MODEL VERIFICATION (1997)

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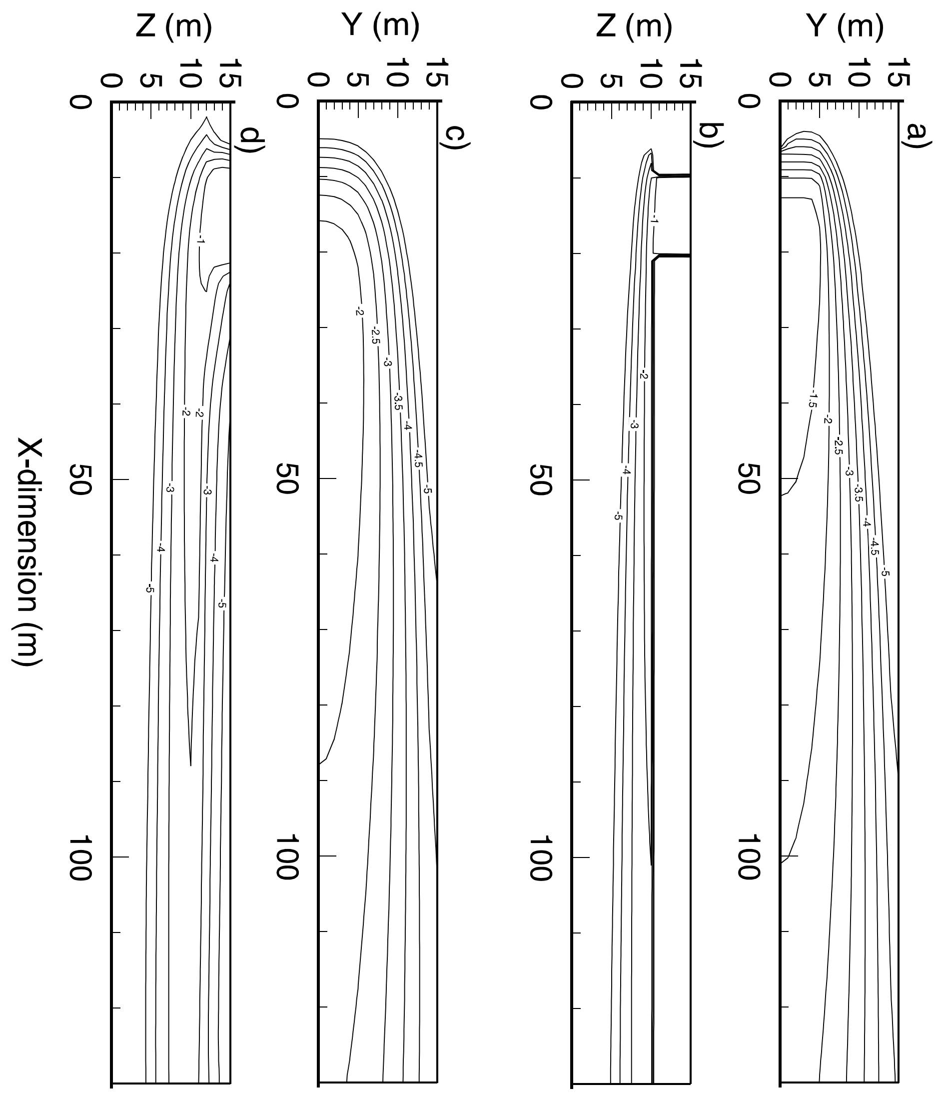

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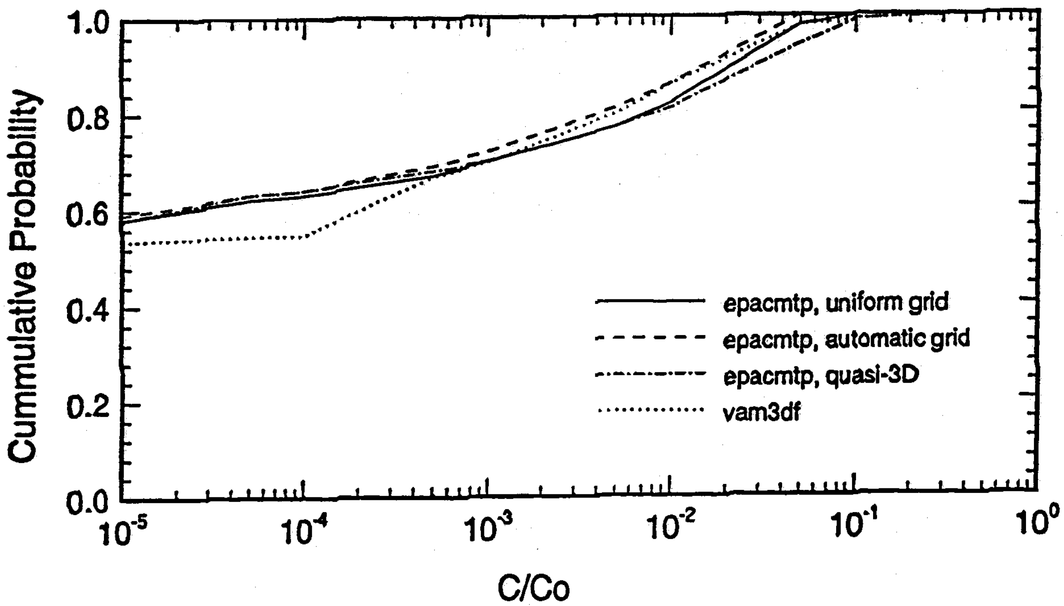

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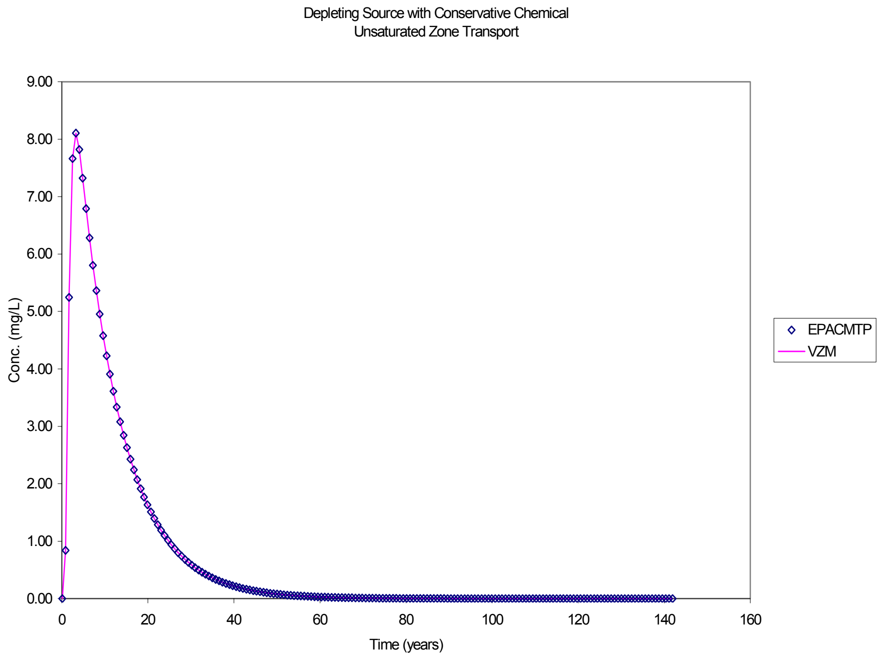
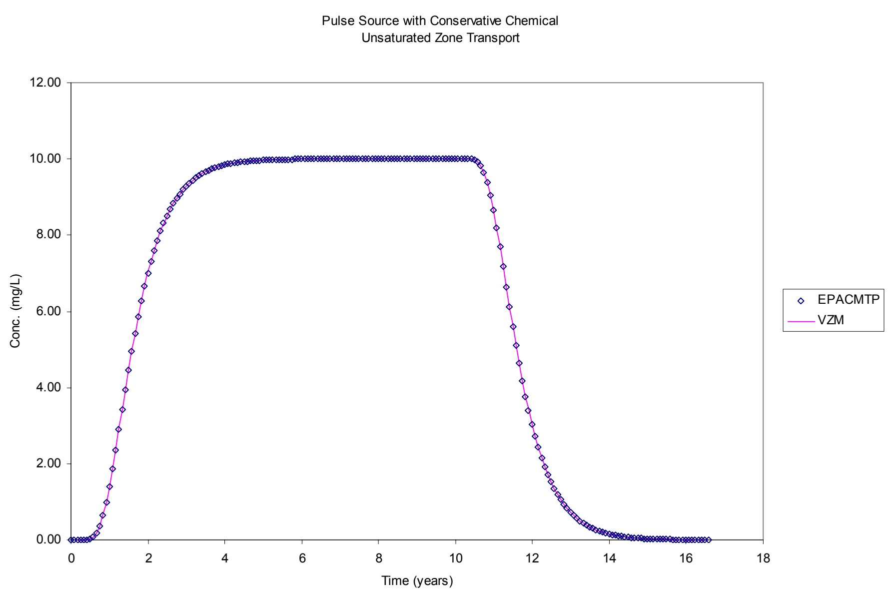


Figure D.G.1 Test Case 1: Exponentially Depleting Source with No Sorption and No Hydrolysis. Comparison of VZM and EPACMTP



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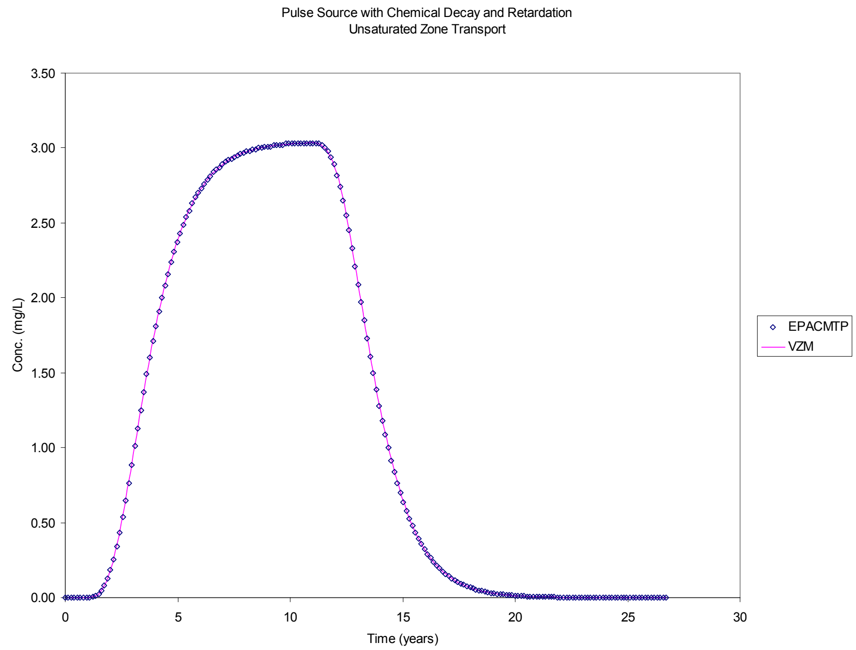

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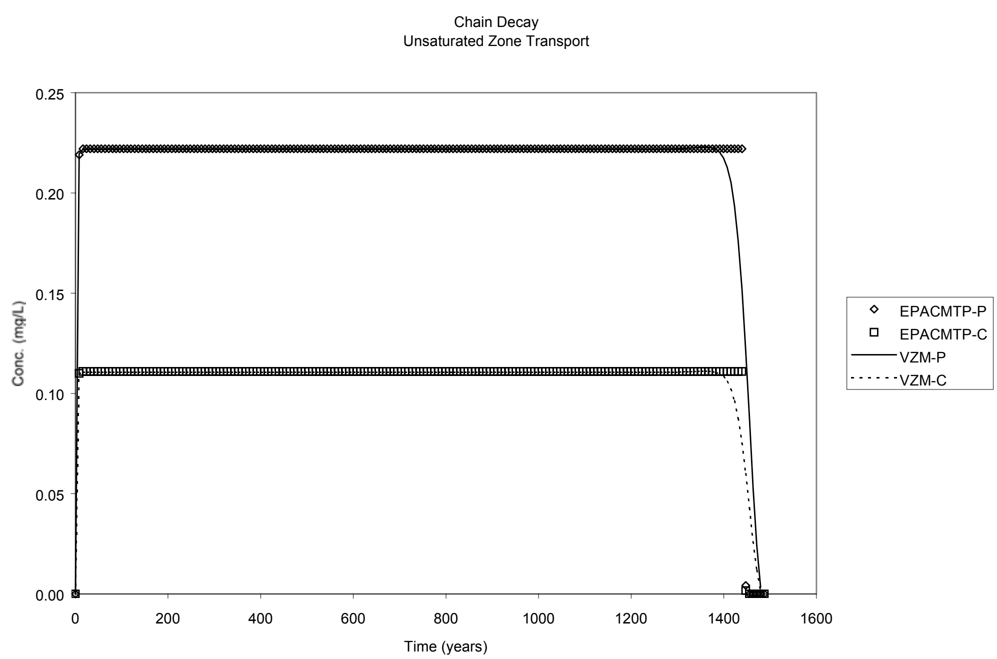

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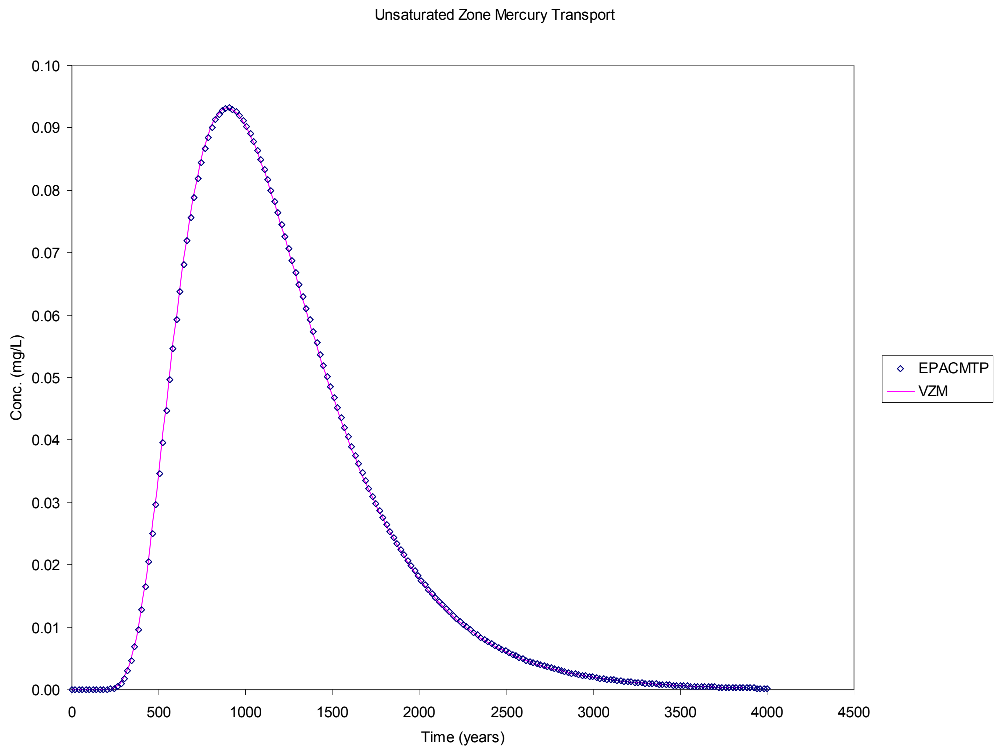

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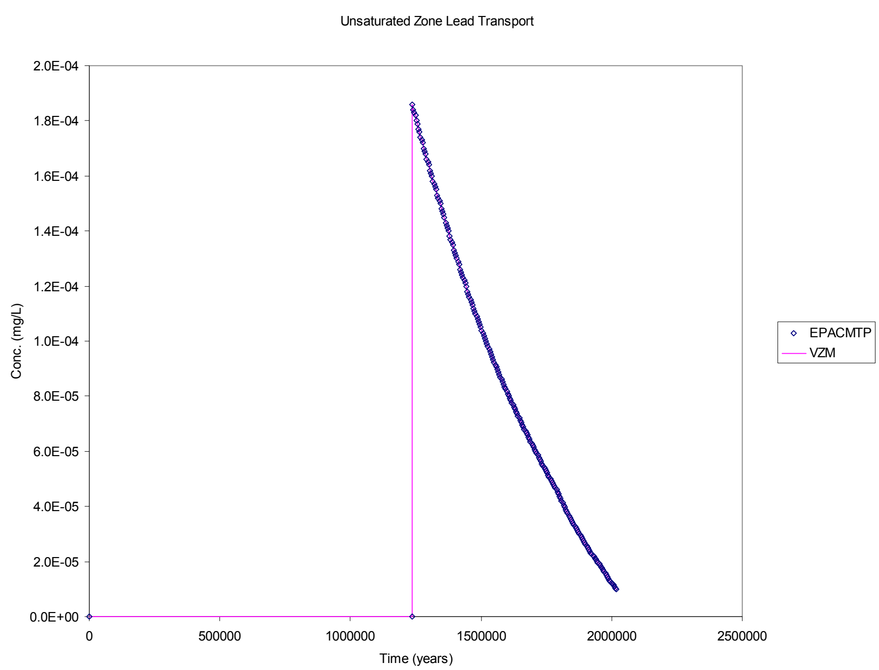

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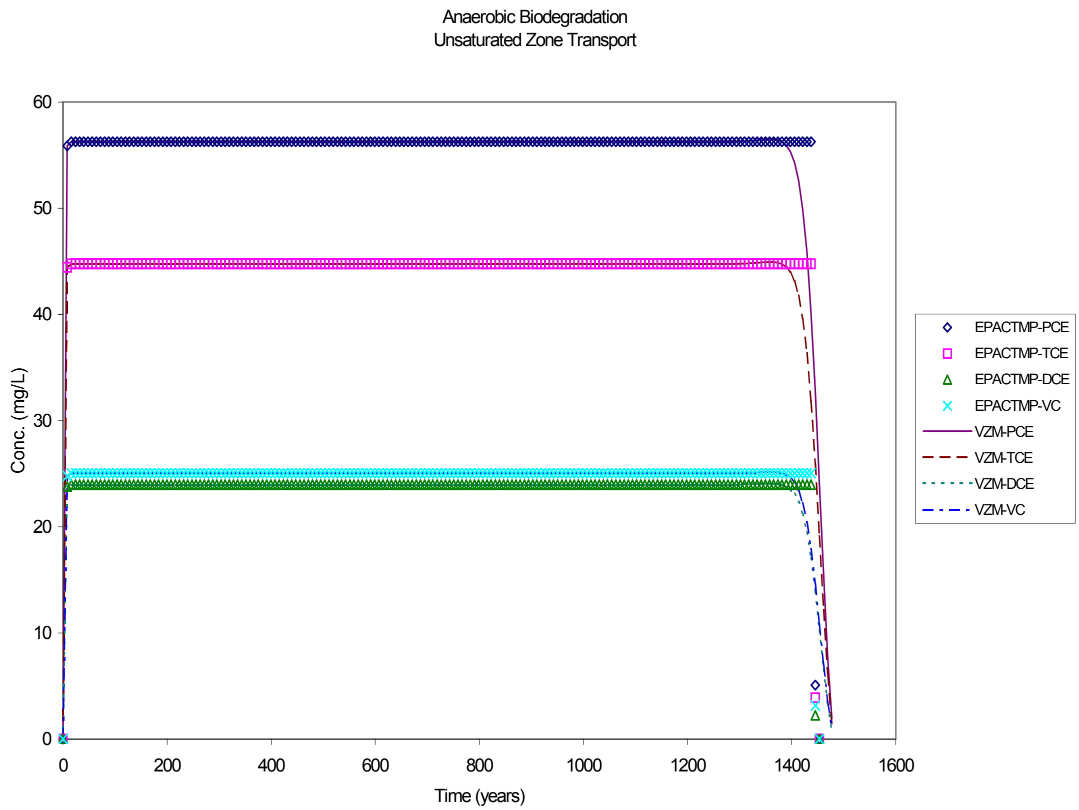

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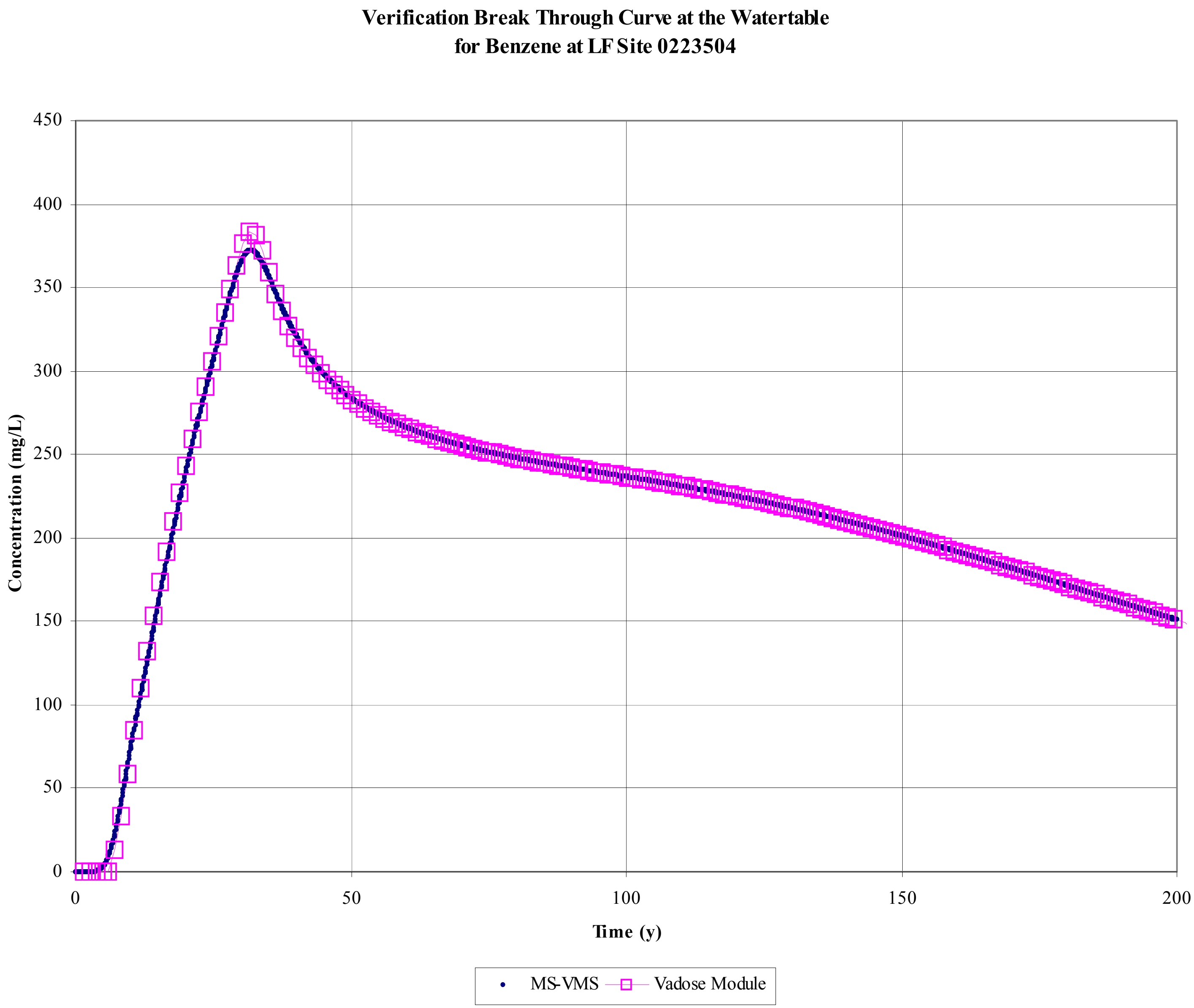
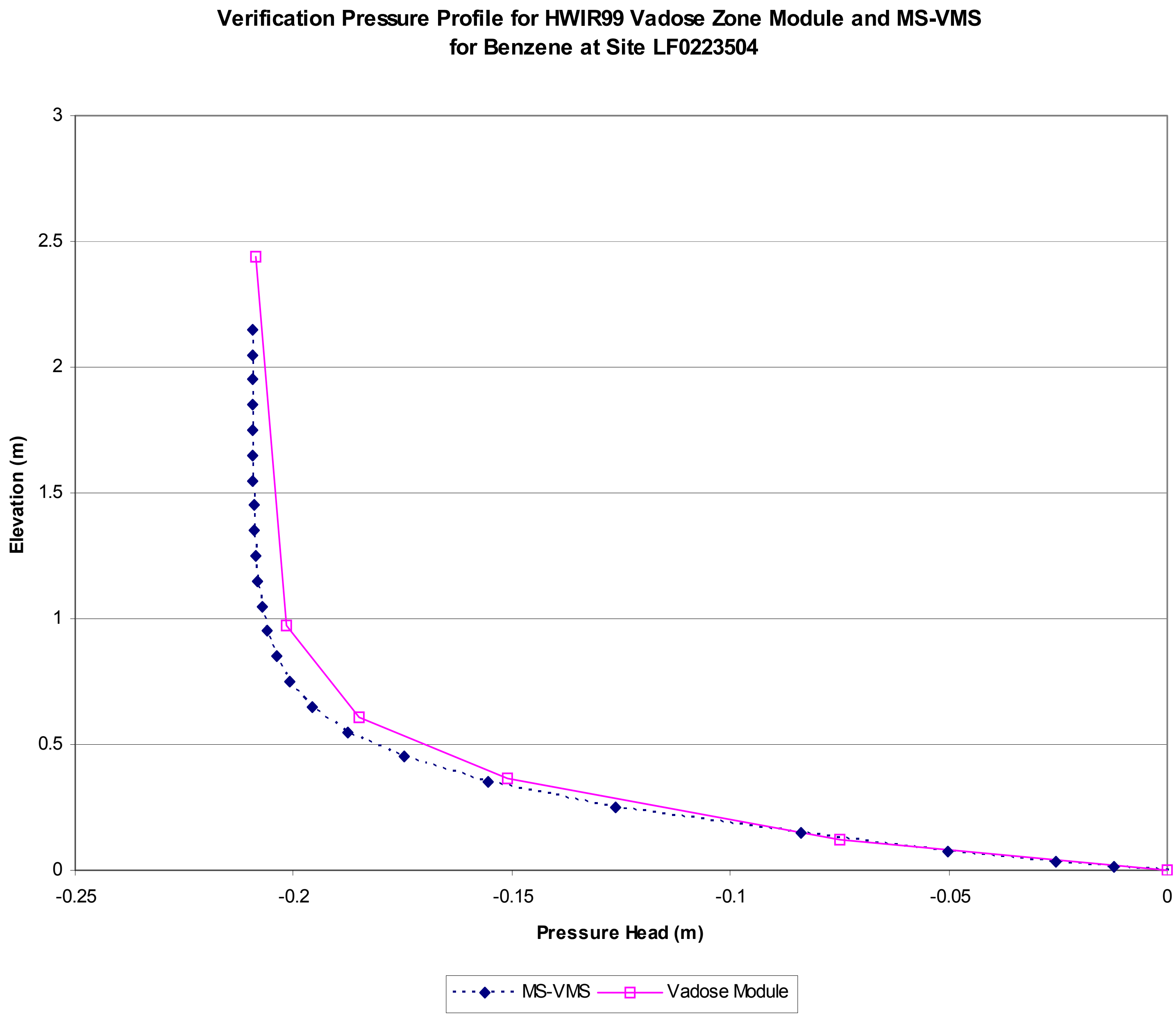


Figure D.G.8 Test Case 7: Breakthrough Curve at the Water Table for Vadoze Zone Module and Verification Code (MS-VMS) at Site LF0223504 for Benzene (Source was Terminated After Time = 200 Years)



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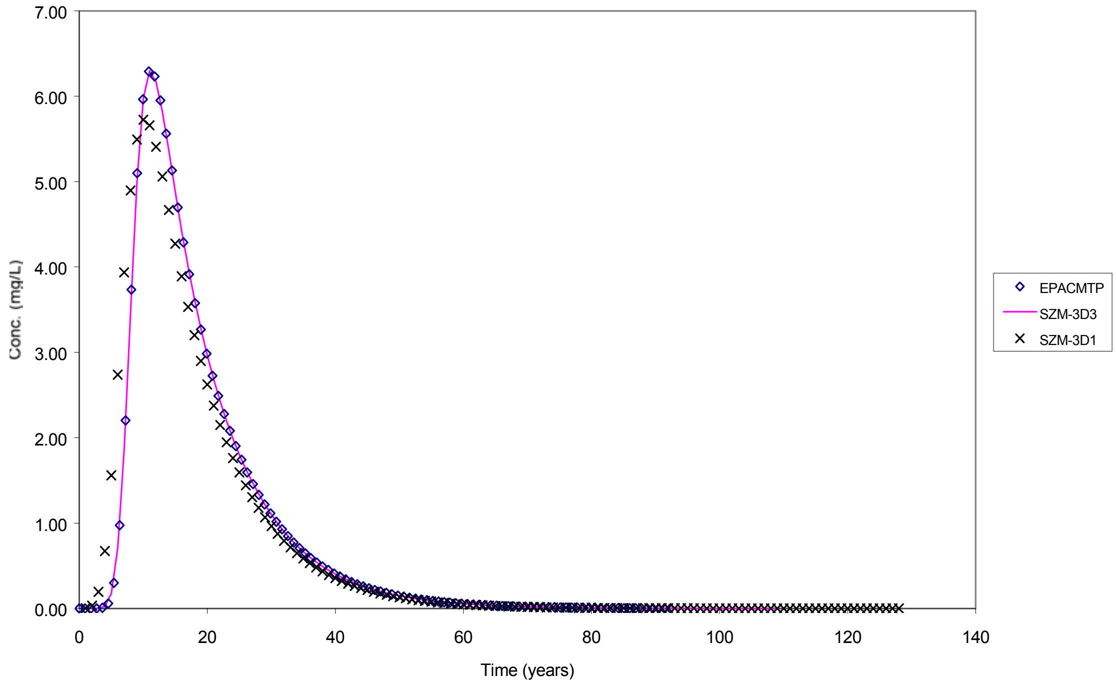


Figure D.H.1 Test Case 1: Exponentially Depleting Source with No Sorption Nor Hydrolysis. Comparison of SZMs and 3-D EPACMTP

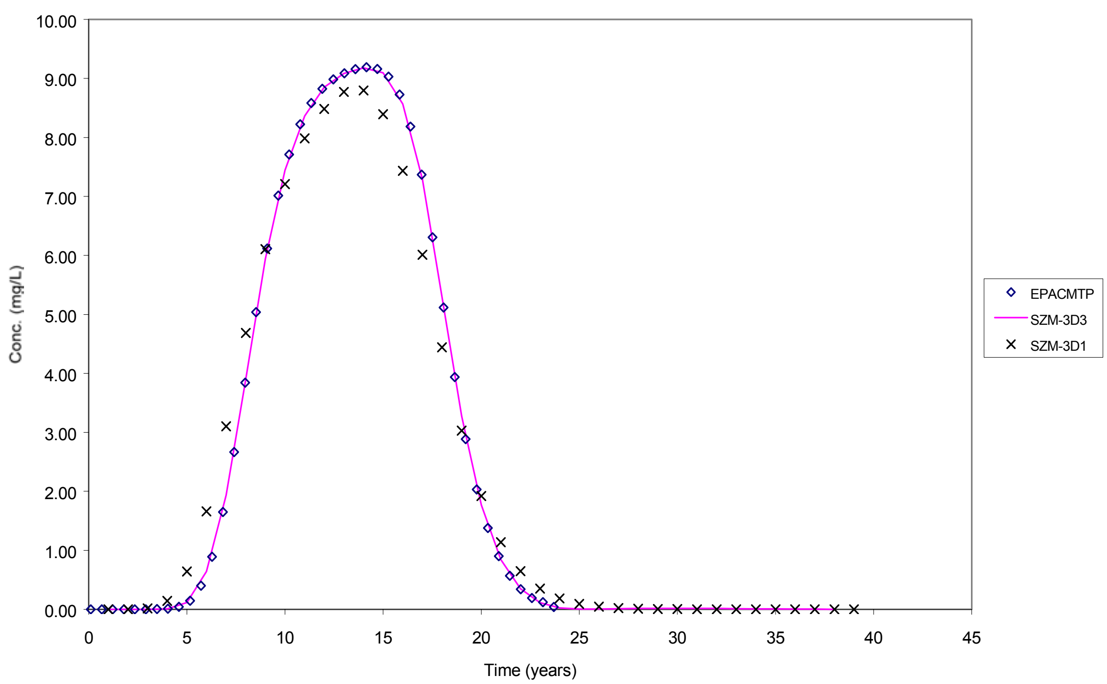


Figure D.H.2 Test Case 2: Constant-concentration Pulse with No Sorption Nor Hydrolysis. Comparison of SZMs and 3-D EPACMTP

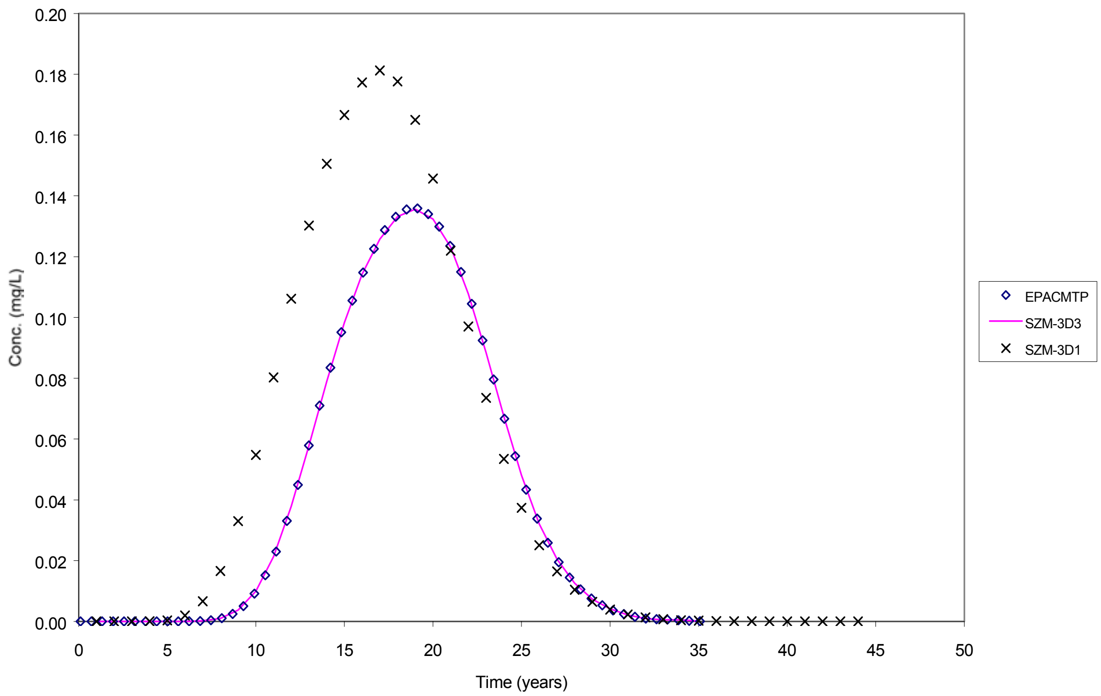
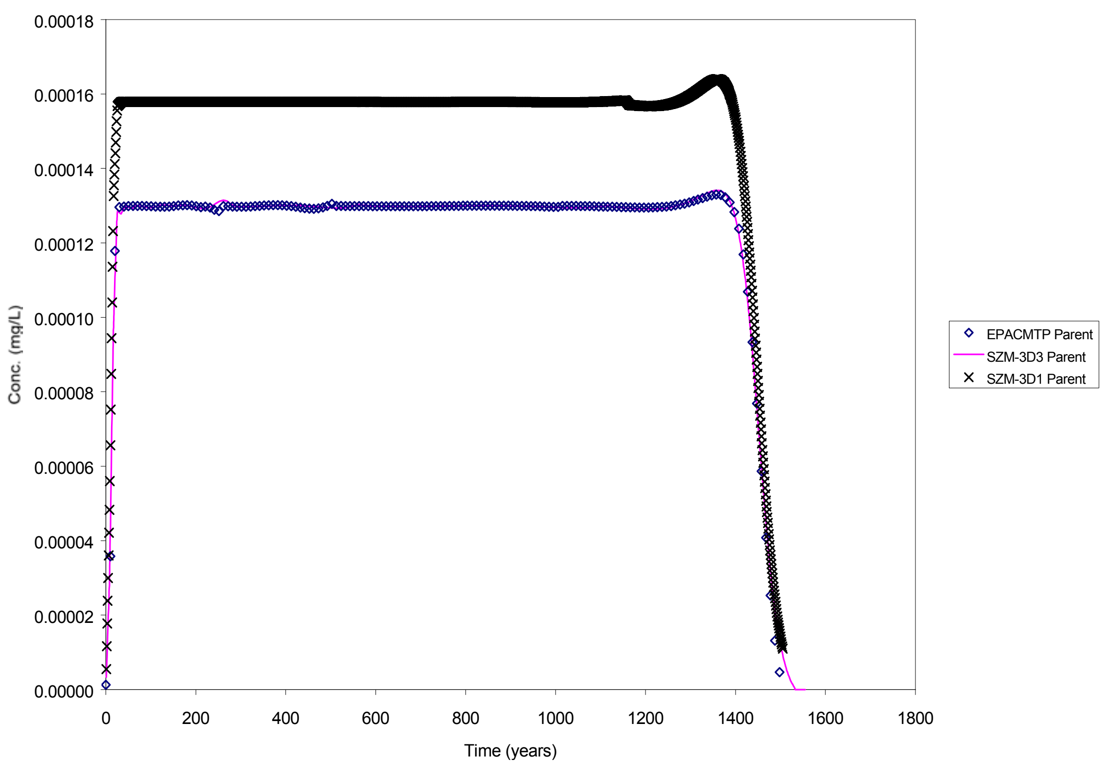


Figure D.H.3 Test Case 3: Constant-concentration Pulse with Sorption and Hydrolysis. Comparison of SZMs and 3-D EPACMTP



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